Symmetry and spontaneous symmetry breaking of the Hubbard model on a square lattice ground state

J. M. P. Carmelo
GCEP-Centre of Physics, University of Minho, Campus Gualtar, P-4710-057 Braga, Portugal
(Dated: 25 March 2010)

In this paper we consider the simplified form that a recently introduced general operator description of the Hubbard model on the square lattice with $N_a^2 \gg 1$ sites, effective transfer integral t, and onsite repulsion U has in a suitable one- and two-electron subspace. Such an operator description is that consistent with the model exact global symmetry recently extended to $SO(3) \times SO(3) \times U(1)$. Our study profits from the rotated-electron occupancy configurations in the original lattice that generate the energy eigenstates being described by occupancy configurations of spin-1/2 spinons in a spin effective lattice, η-spin-1/2 η-spinons in a η-spin effective lattice, and c fermions in a c effective lattice. The latter three types of occupancy configurations refer to state representations of the spin $SU(2)$ symmetry, η-spin $SU(2)$ symmetry, and hidden $U(1)$ symmetry recently found in Ref.[4], respectively. In the limit of very large number of lattice sites $N_a^2 \gg 1$ that such a description refers to the emergence of the above three independent effective lattices simplifies the study of the effects of hole doping on the spin subsystem. In the one- and two-electron subspace the model refers to a square-lattice quantum liquid that plays the same role for the Hubbard model on a square lattice as the Fermi liquid for isotropic three-dimensional correlated perturbative models. There is a large consensus that in the thermodynamic limit $N_a^2 \rightarrow \infty$ long-range antiferromagnetic order occurs in the spin-density $m = 0$ ground state of the half-filled Hubbard model on the square lattice. Here we find that the corresponding spontaneous symmetry breaking lowers the symmetry of such a state from $SO(3) \times SO(3) \times U(1)$ for $N_a^2 \gg 1$ large but finite to $[U(2) \times U(1)]/Z_2^2 \equiv [SO(3) \times U(1) \times U(1)]/Z_2$ for $N_a^2 \rightarrow \infty$. Moreover, we argue that the spin effective lattice being identical to the original lattice is a necessary condition for the occurrence of ground-state long-range antiferromagnetic order in the limit $N_a^2 \rightarrow \infty$. Consistently, strong evidence is provided that for very small hole concentration $0 < x \ll 1$ the ground state has a short-range incommensurate-spiral spin order. (The related investigations of Ref.[19] provide evidence that a spin short-range order exists for $0 < x < x_*$, whereas for $x > x_*$ the ground state is a spin disordered state. Here $x_* > 0.23$ for approximately $U/4t > 1.3$.) Our results are of interest both for condensed-matter systems and ultra-cold fermionic atoms on an optical square lattice. Elsewhere evidence is provided that upon addition of a weak three-dimensional uniaxial anisotropy perturbation to the square-lattice quantum liquid, its short-range spin order coexists for $N_a^2 \rightarrow \infty$, low temperatures, and a well-defined range of finite hole concentrations with a long-range superconducting order.

PACS numbers: 71.10.Fd, 71.10.+w, 71.27.+a, 71.10.Hf, 71.30.+h

I. INTRODUCTION

The Hubbard model on a square lattice is the simplest toy model for describing the effects of electronics correlations in the high-T_c superconductors[1,2] and their Mott-Hubbard insulators parent compounds[3]. In the case of such superconductors, addition of a weak three-dimensional (3D) uniaxial anisotropy perturbation associated with a small effective transverse transfer integral $t_\perp$ is required to capture some of the basic properties of their physics.

The studies of this paper focus on the model on a square lattice. It has no exact solution, so that many open questions about its properties remain unsolved. A recent exact result, which applies to the model on any bipartite lattice[4], is that for on-site repulsion $U > 0$ its global symmetry is $SO(3) \times SO(3) \times U(1) = [SO(4) \times U(1)]/Z_2$. That is an extension of the model well-known $SO(4)$ symmetry[5,6], which becomes explicit provided that one describes the problem in terms of the rotated electrons obtained from the electrons by any of the unitary transformations of the type considered in Refs.[4,7]. Another exact result useful for the studies of this paper is that the ground state of the repulsive half-filled Hubbard model on a bipartite lattice is for finite number of lattice sites and spin density $m = 0$ a spin singlet[5].

The model can be experimentally realized with unprecedented precision in systems of ultra-cold fermionic atoms on an optical lattice with any geometry[8,9]. In the experimental context of cold-fermion optical lattices, Ref.[10] discusses the possibilities to approach the pseudogap or ordered phases by manipulating the scattering length or the strength of the laser-induced lattice potential. In turn, the large square lattices considered in Ref.[11] for the half-filled model provide improved resolution of the Greens function in momentum space, allowing a more quantitative comparison with time-of-flight optical lattice experiments. Such large scale determinant quantum Monte Carlo (DQMC) calculations provide as well useful information on the effective bandwidth, momentum distribution, and magnetic correlations of

the half-lling model.

A. The model

The studies of this paper profit from the simplified form that the general description of the Hubbard model on the square lattice with $N_a^2 \equiv [N_a]^2 \gg 1$ sites, effective nearest-neighbor transfer integral t, and onsite repulsion U introduced in Ref.[12] has in a suitable one- and two-electron subspace considered below. The hole concentration and spin density read $x = [N_a^2 - N]/N_a^2$ and $m = [N_\uparrow - N_\downarrow]/N_a^2$, respectively. The model on such a lattice with spacing a, $N_a \gg 1$ even, and lattice edge length $L = N_a\, a$ is given by,

$$\hat{H} = t\,\hat{T} + U\,[N_a^2 - \hat{Q}]/2\,; \quad \hat{T} = -\sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} [c^\dagger_{\vec{r}_j,\sigma}\, c_{\vec{r}_{j'},\sigma} + h.c.]\,; \quad \hat{Q} = \sum_{j=1}^{N_a^2} \sum_{\sigma=\uparrow,\downarrow} n_{\vec{r}_j,\sigma}\,(1 - n_{\vec{r}_j,-\sigma})\,. \tag{1}$$

Here $\hat{T}$ is the kinetic-energy operator in units of t and $\hat{Q}$ is the operator that counts the number of electron singly occupied sites so that the operator $\hat{D} = [\hat{N} - \hat{Q}]/2$ counts the number of electron doubly occupied sites, $n_{\vec{r}_j,\sigma} = c^\dagger_{\vec{r}_j,\sigma} c_{\vec{r}_j,\sigma}$ where $-\sigma = \uparrow$ (and $-\sigma = \downarrow$) for $\sigma = \downarrow$ (and $\sigma = \uparrow$), $\hat{N} = \sum_\sigma \hat{N}_\sigma$, and $\hat{N}_\sigma = \sum_{j=1}^{N_a^2} n_{\vec{r}_j,\sigma}$.

The kinetic-energy operator $\hat{T}$ given in Eq. (1) can be expressed in terms of the operators,

$$\begin{aligned}
\hat{T}_0 &= -\sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} [n_{\vec{r}_j,-\sigma}\, c^\dagger_{\vec{r}_j,\sigma}\, c_{\vec{r}_{j'},\sigma}\, n_{\vec{r}_{j'},-\sigma} + (1 - n_{\vec{r}_j,-\sigma})\, c^\dagger_{\vec{r}_j,\sigma}\, c_{\vec{r}_{j'},\sigma}\, (1 - n_{\vec{r}_{j'},-\sigma})]\,, \\
\hat{T}_{+1} &= -\sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} n_{\vec{r}_j,-\sigma}\, c^\dagger_{\vec{r}_j,\sigma}\, c_{\vec{r}_{j'},\sigma}\, (1 - n_{\vec{r}_{j'},-\sigma})\,, \\
\hat{T}_{-1} &= -\sum_{\langle \vec{r}_j \vec{r}_{j'} \rangle} \sum_{\sigma} (1 - n_{\vec{r}_j,-\sigma})\, c^\dagger_{\vec{r}_j,\sigma}\, c_{\vec{r}_{j'},\sigma}\, n_{\vec{r}_{j'},-\sigma}\,,
\end{aligned} \tag{2}$$

as $\hat{T} = \hat{T}_0 + \hat{T}_{+1} + \hat{T}_{-1}$. As discussed in Refs.[4,12,13], these three kinetic operators play an important role in the physics. The operator $\hat{T}_0$ does not change electron double occupancy whereas the operators $\hat{T}_{+1}$ and $\hat{T}_{-1}$ do it by $+1$ and -1, respectively.

B. The general rotated-electron operator description

The general operator representation introduced in Ref.[12] applies for $N_a^2 \gg 1$ and refers to suitable quantum objects whose occupancy configurations generate the state representations of the group $SO(3) \times SO(3) \times U(1)$. Addition of chemical-potential and magnetic-field operator terms to the Hamiltonian lowers the model symmetry. Such terms commute with it so that its $4^{N_a^2}$ momentum and energy eigenstates correspond to representations of that group for all values of x and m. It is shown in such a reference that all the physics of the model in the whole Hilbert space can be obtained from that of the model in the subspace spanned by the lowest-weight states (LWSs) of both the η-spin $SU(2)$ and spin $SU(2)$ algebras. In this paper we profit from the simpler properties that the general operator description introduced in Ref.[12] has in a suitable *one- and two-electron subspace*. That subspace is spanned by a well-defined set of energy eigenstates, which for $U/4t > 0$ are generated by simple momentum occupancy configurations of spin-less charge objects and spin-singlet objects, respectively.

The general description introduced in Ref.[12] refers for $U/4t > 0$ to a particular choice of the complete set of $4^{N_a^2}$ energy, momentum, η-spin, η-spin projection, spin, and spin-projection eigenstates $\{|\Psi_{U/4t}\rangle\}$. In the limit $U/4t \rightarrow \infty$ such states correspond to one of the many choices of sets $\{|\Psi_\infty\rangle\}$ of $4^{N_a^2}$ $U/4t$-infinite energy eigenstates. For the choice corresponding to the description of Ref.[12] there exists exactly one unitary operator $\hat{V} = \hat{V}(U/4t)$ such that $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$. The point is that for most choices of the set of energy eigenstates $\{|\Psi_\infty\rangle\}$ the corresponding states $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$ are not energy eigenstates for $U/4t > 0$. For the description introduced in that reference such states are energy eigenstates. The corresponding unitary operator $\hat{V} = \hat{V}(U/4t)$ and the rotated-electron operators,

$$\tilde{c}^\dagger_{\vec{r}_j,\sigma} = \hat{V}^\dagger\, c^\dagger_{\vec{r}_j,\sigma}\, \hat{V}\,; \quad \tilde{c}_{\vec{r}_j,\sigma} = \hat{V}^\dagger\, c_{\vec{r}_j,\sigma}\, \hat{V}\,; \quad \tilde{n}_{\vec{r}_j,\sigma} = \tilde{c}^\dagger_{\vec{r}_j,\sigma}\, \tilde{c}_{\vec{r}_j,\sigma}\,, \tag{3}$$

play a central role in that description. The states $|\Psi_{U/4t}\rangle = \hat{V}^\dagger |\Psi_\infty\rangle$ (one for each value of $U/4t > 0$) that are generated from the same initial state $|\Psi_\infty\rangle$ belong to the same V *tower*.

Any operator $\hat{O}$ can be written in terms of rotated-electron creation and annihilation operators as,

$$\hat{O} = \hat{V}\,\tilde{O}\,\hat{V}^{\dagger} = \tilde{O} + [\tilde{O},\,\hat{S}\,] + \frac{1}{2}\,[[\tilde{O},\,\hat{S}\,],\,\hat{S}\,] + ... = \tilde{O} + [\tilde{O},\,\tilde{S}\,] + \frac{1}{2}\,[[\tilde{O},\,\tilde{S}\,],\,\tilde{S}\,] + ...\,,$$
$$\hat{S} = -\frac{t}{U}\,\left[\hat{T}_{+1} - \hat{T}_{-1}\right] + \mathcal{O}(t^2/U^2)\,; \quad \tilde{S} = -\frac{t}{U}\,\left[\tilde{T}_{+1} - \tilde{T}_{-1}\right] + \mathcal{O}(t^2/U^2)\,. \tag{4}$$

Here the operator $\tilde{O} = \hat{V}^{\dagger}\,\hat{O}\,\hat{V}$ has the same expression in terms of rotated-electron creation and annihilation operators as $\hat{O}$ in terms of electron creation and annihilation operators, respectively. The operator $\hat{S}$ appearing in Eq. (4) is related to the unitary operator as $\hat{V}^{\dagger} = e^{\hat{S}}$ and $\hat{V} = e^{-\hat{S}}$. Since for finite $U/4t$ values the Hamiltonian $\hat{H}$ of Eq. (1) does not commute with the unitary operator $\hat{V} = e^{-\hat{S}}$, when expressed in terms of rotated-electron creation and annihilation operators it has an infinite number of terms. According to Eq. (4) it then reads,

$$\hat{H} = \hat{V}\,\tilde{H}\,\hat{V}^{\dagger} = \tilde{H} + [\tilde{H},\,\tilde{S}\,] + \frac{1}{2}\,[[\tilde{H},\,\tilde{S}\,],\,\tilde{S}\,] + ...\,. \tag{5}$$

The commutator $[\tilde{H},\,\tilde{S}\,]$ does not vanish except for $U/4t \rightarrow \infty$ so that $\hat{H} \neq \tilde{H}$ for finite values of $U/4t$.

For $U/4t$ very large the Hamiltonian of Eq. (5) corresponds in terms of rotated-electron creation and annihilation operators to a simple rotated-electron $t-J$ model. In turn, the higher-order t/U terms become increasingly important upon decreasing $U/4t$. They generate effective rotated-electron hopping between second, third, and more distant neighboring sites. Indeed, the products of the kinetic operators $\tilde{T}_0$, $\tilde{T}_{+1}$, and $\tilde{T}_{-1}$ contained in the higher-order terms of $\tilde{S} = -(t/U)\,[\tilde{T}_{+1} - \tilde{T}_{-1}] + \mathcal{O}(t^2/U^2)$ also appear in the Hamiltonian expression (5) in terms of rotated-electron creation and annihilation operators of Eq. (3). In spite of the operators $\tilde{T}_0$, $\tilde{T}_{+1}$, and $\tilde{T}_{-1}$ generating only rotated-electron hopping between nearest-neighboring sites, their products generate effective hopping between for instance second and third neighboring sites. For instance, the Hamiltonian terms generated up to fourth order in t/U are within a unitary transformation the equivalent to the $t-J$ model with ring exchange and various correlated hoppings[13]. The real-space distance in units of the lattice spacing a associated with the effective hopping between second and third neighboring sites is for the model on the square lattice $\sqrt{2}\,a$ and $2\,a$, usually associated with transfer integrals t' and t'', respectively. For instance, for the half filled Hubbard model on the square lattice in the subspace with both vanishing rotated-electron double occupancy and vanishing rotated-hole double occupancy the interactions can be expressed completely by spin operators. The corresponding Hamiltonian expression is given below in Section III-B up to fifth order in t/U. Some of the interactions in spin space in its t^4/U^3 terms refer indeed to pair of spins at second and third neighboring sites.

It follows that when expressed in terms of the rotated-electron operators emerging from the specific unitary transformation considered above the simple Hubbard model (1) as given in Eq. (5) contains Hamiltonian terms associated with higher-order contributions. Those can be effectively described by transfer integrals t', t'', and of higher order. For hole concentration equal to or larger than zero both the model ground state and the excited states that span the one- and two-electron subspace considered below have vanishing rotated-electron double occupancy. Fortunately, for intermediate and large values of $U/4t$ obeying approximately the inequality $U/4t \geq u_0 \approx 1.3$ and thus $t/U < 0.2$, besides the original nearest-neighboring hopping processes only those involving second and third neighboring sites are relevant for the square-lattice quantum liquid. That quantum liquid refers to the Hamiltonian of Eqs. (1) and (5) in the one- and two-electron subspace. The value $U/4t = u_0 \approx 1.302$ is that at which an important energy scale Δ_0 whose $U/4t$ dependence is studied below in Section III-C reaches its maximum magnitude.

Hence for approximately $U/4t \geq u_0$, out of the infinite terms on the right-hand-side of Eq. (5) only the first few Hamiltonian terms play an active role in the physics of the Hubbard model on the square lattice in the one- and two-electron subspace. Therefore, for intermediate and large values of $U/4t$ such a square-lattice quantum liquid can be mapped onto an effective $t-J$ model on a square lattice with t, $t' = t'(U/4t)$, and $t'' = t''(U/4t)$ transfer integrals. The role of the processes associated with $t' = t'(U/4t)$ and $t'' = t''(U/4t)$ becomes increasingly important upon decreasing the $U/4t$ value.

C. Three basic objects emerging from the rotated-electron description

In addition to the spin S_s and η-spin S_η associated with the spin $SU(2)$ and η-spin $SU(2)$ symmetries, respectively, of the model global $SO(3)\times SO(3)\times U(1) = [SU(2)\times SU(2)\times U(1)]/Z_2^2$ symmetry, the eigenvalue S_c of the generator of the hidden $U(1)$ symmetry found in Ref.[4] plays an important role in the general rotated-electron description of Ref.[12]. It is such that $2S_c$ is the number of rotated-electron singly occupied sites, which is a good quantum number for $U/4t > 0$. We denote the η-spin and spin projection by $S_\eta^{x_3} = -[N_a^2 - N]/2$ and $S_s^{x_3} = -[N_\uparrow - N_\downarrow]/2$, respectively.

That the global symmetry of the Hubbard model on a bipartite lattice is $[SU(2) \times SU(2) \times U(1)]/Z_2^2$ rather than $SU(2) \times SU(2) \times U(1)$ is due to only state representations such that $2S_\eta$, $2S_s$, and $2S_c$ are simultaneously even or odd integer numbers being allowed[4]. The group $SU(2) \times SU(2) \times U(1)$ has the same seven generators but four times more representations than the group $SO(3) \times SO(3) \times U(1)$.

Studies of the Hubbard model on the square lattice that rely on its transformation properties under symmetry operations[14] should be extended to account for the new hidden $U(1)$ symmetry recently found in Ref.[4]. Indeed that the global symmetry of the Hubbard model on a square lattice and all other bipartite lattices is larger than $SO(4)$ and given by $SO(3) \times SO(3) \times U(1)$ is expected to have important physical consequences. In the case of the one-dimensional (1D) bipartite lattice the model has an exact solution[15–17]. The main reason why its solution by the algebraic Bethe-ansatz inverse scattering method[17] was achieved only thirty years after that of the coordinate Bethe ansatz[15,16] is that it was expected that the charge and spin monodromy matrices had the same traditional ABCD form, found previously for the related 1D isotropic spin 1/2 Heinsenberg model[18]. Such an expectation was that consistent with the occurrence of a spin $SU(2)$ symmetry and a charge (and η-spin) $SU(2)$ symmetry known long ago[6], associated with a global $SO(4) = [SU(2) \times SU(2)]/Z_2$ symmetry. If that was the whole global symmetry of the 1D Hubbard model, the charge and spin sectors would be associated with the η-spin $SU(2)$ symmetry and spin $SU(2)$ symmetry, respectively. A global $SO(4) = [SU(2) \times SU(2)]/Z_2$ symmetry would then imply that the charge and spin monodromy matrices had indeed the same Faddeev-Zamolodchikov ABCD form. Fortunately, Martins and Ramos used an appropriate representation of the charge and spin monodromy matrices, which allows for possible *hidden symmetries*[17]. For the particular case of the bipartite 1D lattice the results of Ref.[4] reveal that the hidden symmetry beyond $SO(4)$ is the charge global $U(1)$ symmetry found in that reference. For $U/4t > 0$ the model charge and spin degrees of freedom are then associated with $U(2) = SU(2) \times U(1)$ and $SU(2)$ symmetries, rather than with two $SU(2)$ symmetries, respectively. The occurrence of such charge $U(2) = SU(2) \times U(1)$ symmetry and spin $SU(2)$ symmetry is behind the different ABCDF and ABCD forms of the charge and spin monodromy matrices of Ref.[17], respectively.

Addition of chemical-potential and magnetic-field operator terms to the Hamiltonian (1) lowers its symmetry. As mentioned above, such terms commute with it so that the global symmetry being $[SU(2) \times SU(2) \times U(1)]/Z_2^2 = SO(3) \times SO(3) \times U(1)$ implies that a set of $4^{N_a^2}$ independent rotated-electron occupancy configurations generate the corresponding state representations of that global symmetry for all values of the electronic density $n = (1 - x)$ and spin density m. Consistently, in Ref.[4] it is confirmed that the total number of such independent representations equals indeed the Hilbert-space dimension $4^{N_a^2}$. The rotated electron occupancy configurations that generate such state representations are simpler to describe in terms of those of suitable related quantum objects. The eigenvalue S_c of the new hidden $U(1)$ symmetry controls the numbers of such objects, which are as well good quantum numbers. Indeed the investigations of Ref.[12] reveal the emergence within the rotated-electron description of three basic quantum objects: $M_s = 2S_c$ spin-1/2 spinons, $M_\eta = [N_a^2 - 2S_c]$ η-spin-1/2 η-spinons, and $N_c = 2S_c$ spin-less and η-spin-less charge c fermions. The latter live on a lattice with $N_a^2 = [N_c + N_c^h]$ sites identical to the original lattice. Here $N_c^h = [N_a^2 - 2S_c]$ gives the number of c fermion holes.

The relation of such objects to the rotated electrons is as follows. The $M_s = 2S_c$ spin-1/2 spinons describe the spin degrees of freedom of the $2S_c$ rotated electrons that singly occupied sites. The $M_\eta = [N_a^2 - 2S_c]$ η-spin-1/2 η-spinons describe the η-spin degrees of freedom of the $[N_a^2 - 2S_c]$ sites doubly occupied and unoccupied by rotated electrons. Specifically, the η-spinons of η-spin projection $-1/2$ and $+1/2$ refer to the sites doubly occupied and unoccupied, respectively, by rotated electrons. The counting of the number of spinon and η-spinon independent occupancy configurations is an exercise fulfilled in Ref.[4]. However, the internal structure of the specific spinon and η-spinon occupancy configurations of the $4^{N_a^2}$ $U/4t > 0$ energy eigenstates associated with the Ref.[12] description is a complex problem, which partially simplifies in the one- and two-electron subspace considered below. In turn, in each rotated-electron configuration of a $U/4t > 0$ energy eigenstate, the $N_c = 2S_c$ c fermions exactly occupy the same sites as the $2S_c$ rotated electrons that singly occupy sites. Furthermore, the $N_c^h = [N_a^2 - 2S_c]$ sites unoccupied by c fermions are those doubly occupied and unoccupied by the rotated electrons. The electronic charges of the $2S_c$ rotated electrons that singly occupy sites are carried by the $N_c = 2S_c$ c fermions whereas their spins are carried by the $M_s = 2S_c$ spin-1/2 spinons.

For the general description of Ref.[12] the rotated-electron occupancy configurations referring to (i) the spin degrees of freedom of the singly occupied and (ii) the η-spin degrees of freedom of the unoccupied and doubly-occupied sites are independent. They correspond to the state representations of the spin $SU(2)$ symmetry $M_s = 2S_c$ spin-1/2 spinons and η-spin $SU(2)$ symmetry $M_\eta = 2S_c^h$ η-spin-1/2 η-spinons, respectively. In turn, the $U(1)$ symmetry state representations refer to the relative occupancy configurations of the $2S_c$ rotated-electron singly-occupied sites and $2S_c^h$ rotated-electron unoccupied and doubly-occupied sites. Those correspond to the c fermion occupancy configurations.

Within the LWS representation of the general operator description introduced in Ref.[12], the c fermion creation

operator has the following expression in terms of the rotated-electron operators of Eq. (3),

$$f^{\dagger}_{\vec{r}_j,c} = \tilde{c}^{\dagger}_{\vec{r}_j,\uparrow}\,(1-\tilde{n}_{\vec{r}_j,\downarrow}) + e^{i\vec{\pi}\cdot\vec{r}_j}\,\tilde{c}_{\vec{r}_j,\uparrow}\,\tilde{n}_{\vec{r}_j,\downarrow}\,; \quad f^{\dagger}_{\vec{q}_j,c} = \frac{1}{\sqrt{N_a^2}}\sum_{j'=1}^{N_a^2} e^{+i\vec{q}_j\cdot\vec{r}_{j'}}\,f^{\dagger}_{\vec{r}_{j'},c}\,. \tag{6}$$

Here we have introduced the corresponding c fermion momentum-dependent operators as well and $e^{i\vec{\pi}\cdot\vec{r}_j}$ is ± 1 depending on which sub-lattice site $\vec{r}_j$ is on. The use of Eq. (3) allows the expression of the c fermion operators (6) in terms of electron operators. This involves the electron - rotated-electron unitary operator $\hat{V}$. The c momentum band is studied in Ref.[19] and has the same shape and momentum area as the electronic first-Brillouin zone.

In turn, the three spinon local operators $s^{l}_{\vec{r}_j}$ and three η-spinon local operators $p^{l}_{\vec{r}_j}$ such that $l = \pm, z$ are given by,

$$s^{l}_{\vec{r}_j} = n_{\vec{r}_j,c}\,q^{l}_{\vec{r}_j}\,; \quad p^{l}_{\vec{r}_j} = (1-n_{\vec{r}_j,c})\,q^{l}_{\vec{r}_j}\,, \;\; l = \pm, x_3\,. \tag{7}$$

Here $q^{x_3}_{\vec{r}_j}$ and $q^{\pm}_{\vec{r}_j} = q^{x_1}_{\vec{r}_j} \pm i\,q^{x_2}_{\vec{r}_j}$ are the rotated quasi-spin operators $q^{l}_{\vec{r}_j} = s^{l}_{\vec{r}_j} + p^{l}_{\vec{r}_j}$. (We denote the Cartesian coordinates by x_1, x_2, x_3.) In addition,

$$n_{\vec{r}_j,c} = f^{\dagger}_{\vec{r}_j,c}\,f_{\vec{r}_j,c}\,, \tag{8}$$

is the c fermion local density operator. In terms of rotated-electron creation and annihilation operators the rotated quasi-spin operators read,

$$q^{+}_{\vec{r}_j} = s^{+}_{\vec{r}_j} + p^{+}_{\vec{r}_j} = (\tilde{c}^{\dagger}_{\vec{r}_j,\uparrow} - e^{i\vec{\pi}\cdot\vec{r}_j}\,\tilde{c}_{\vec{r}_j,\uparrow})\,\tilde{c}_{\vec{r}_j,\downarrow}\,; \quad q^{-}_{\vec{r}_j} = (q^{+}_{\vec{r}_j})^{\dagger}\,; \quad q^{x_3}_{\vec{r}_j} = s^{x_3}_{\vec{r}_j} + p^{x_3}_{\vec{r}_j} = \frac{1}{2} - \tilde{n}_{\vec{r}_j,\downarrow}\,. \tag{9}$$

D. Two qualitatively different types of spinon (and η-spinon) configurations and our notation

An important result of Ref.[12] is that a well-defined number of spin-1/2 spinons and η-spin-1/2 η-spinons remain invariant under the electron - rotated-electron unitary transformation. We call those independent spinons and independent η-spinons, respectively. In the one- and two-electron subspace considered in this paper there are no η-spin-projection $-1/2$ η-spinons. The independent spinons and the independent η-spin-projection $+1/2$ η-spinons have vanishing energy and momentum. There are no independent spinons in $m = 0$ ground states.

The spinons that are not invariant under the electron - rotated-electron unitary transformation are confined within spin-neutral 2ν-spinon composite $s\nu$ fermions. Here $\nu = 1, 2, ...$ is the number of spinon pairs confined within a spin-neutral 2ν-spinon composite $s\nu$ fermion. The description of Ref.[12] used in our studies refers to a number of sites $N_a^2 \gg 1$ very large but finite. Within such a description all $m = 0$ ground-state spinons are confined within spin-neutral two-spinon $s1$ fermions. The condition that in an excited state spinons are deconfined is that they are invariant under the electron - rotated-electron unitary transformation. For instance, a spin-triplet excited state involves two independent spinons that correspond to an isolated mode below a continuum of two-$s1$-fermion-hole excitations.

For a given state, the values of the numbers $L_{\eta,\,\pm 1/2}$ of independent $\pm 1/2$ η-spinons and $L_{s,\,\pm 1/2}$ of independent $\pm 1/2$ spinons are fully determined by those of the η-spin S_η and η-spin projection $S^{x_3}_{\eta} = -x\,N_a^2$ and spin S_s and spin projection $S^{x_3}_{s} = -m\,N_a^2$, respectively, as follows,

$$L_\alpha = [L_{\alpha,-1/2} + L_{\alpha,+1/2}] = 2S_\alpha\,; \quad L_{\alpha,\,\pm 1/2} = [S_\alpha \mp S^{x_3}_{\alpha}]\,; \quad \alpha = \eta\,, s\,. \tag{10}$$

The invariance of such independent η-spinons (and spinons) stems from the off diagonal generators of the η-spin (and spin) algebra, which flip their η-spin (and spin), commuting with the unitary operator $\hat{V}$. Hence it follows from Eq. (4) that such generators have for $U/4t > 0$ the same expressions in terms of electron and rotated-electron operators.

Alike the spin-1/2 spinons, the η-spin-1/2 η-spinons that are not invariant under the electron - rotated-electron unitary transformation are confined within η-spin-neutral 2ν-η-spinon composite $\eta\nu$ fermions. Within the notation of Ref.[12] also used in this paper, $\nu = 1, ..., C_\eta$ and $\nu = 1, ..., C_s$ are the numbers of η-spinon and spinon pairs confined within a composite $\eta\nu$ fermion and a $s\nu$ fermion, respectively. Their maximum values C_η and C_s, respectively, are given in Eq. (A5) of Appendix A. In principle there are some occupancy configurations of such objects that generate the exact momentum and energy eigenstates for $U/4t > 0$, yet the detailed internal structure of such configurations is a complex problem[12].

Accordingly to the studies of Ref.[12] that refer to $N_a^2 \gg 1$ very large but finite the $m = 0$ and $x \geq 0$ ground states are spin singlets with $N_{s1} = M_s/2 = S_c = N/2$ two-spinon $s1$ fermions, $N_c = 2S_c = N = (1-x)N_a^2$ c fermions,

$L_{\eta,+1/2} = [N_a^2 - 2S_c] = x\, N_a^2$ η-spinon-projection $+1/2$ independent η-spinons, no independent spinons, no $s\nu$ fermions with $\nu > 1$ spinon pairs, and no $\eta\nu$ fermions. It is found below that for the Hubbard model on the square lattice in the one- and two-electron subspace considered in the studies of this paper only the c fermions and the two-spinon $s1$ fermions play an active role. In the two quantum liquids referring to (i) $x = 0$ and $m = 0$ and (ii) $x > 0$ and $m = 0$, respectively, considered in our studies all the ground-state $M_s = 2S_c$ spinons are for $N_a^2 \gg 1$ very large but finite confined within $N_{s1} = M_s/2$ spin-neutral two-spinon $s1$ fermions. Spinon confinement and the corresponding deconfined degrees of freedom in second-order phase transitions is a problem of physical interest[20–22].

In summary, the degrees of freedom of the rotated-electron occupancy configurations of each of the sets of $N_{a_\eta}^2 = [N_a^2 - 2S_c]$ and $N_{a_s}^2 = 2S_c$ sites of the original lattice that generate the energy eigenstates separate into two types of configurations. A first type of occupancy configurations are those of the c fermions associated with the operators $f^\dagger_{\vec{r}_j,c}$ of Eq. (6) where $j = 1, ..., N_a^2$. Such occupancy configurations correspond to the state representations of the global $U(1)$ symmetry found in Ref.[4]. The c fermions live on a c effective lattice, which is identical to the original lattice. The $N_c = N_{a_s}^2 = 2S_c$ c fermions occupy the sites singly occupied by the rotated electrons. The $N_c^h = N_{a_\eta}^2 = [N_a^2 - 2S_c]$ rotated-electron doubly-occupied and unoccupied sites are those unoccupied by the c fermions. The c fermion occupancy configurations describe the relative positions in the original lattice of the $N_{a_\eta}^2 = [N_a^2 - 2S_c]$ sites of the η-spin effective lattice and $N_{a_s}^2 = 2S_c$ sites of the spin effective lattice.

Consistently, the remaining degrees of freedom of rotated-electron occupancies of the sets of $N_{a_\eta}^2 = [N_a^2 - 2S_c]$ and $N_{a_s}^2 = 2S_c$ original-lattice sites correspond to a second type of occupancy configurations. Those are associated with the η-spin $SU(2)$ symmetry and spin $SU(2)$ symmetry representations, respectively. The occupancy configurations of the set of $N_{a_\eta}^2 = [N_a^2 - 2S_c]$ sites of the η-spin effective lattice and set of $N_{a_s}^2 = 2S_c$ sites of the spin effective lattice are independent. The former configurations refer to the operators $p^l_{\vec{r}_j}$ of Eq. (7), which act only onto the $N_{a_\eta}^2 = [N_a^2 - 2S_c]$ sites of the η-spin effective lattice. The latter configurations correspond to the operators $s^l_{\vec{r}_j}$ given in the same equation, which act onto the $N_{a_s}^2 = 2S_c$ sites of the spin effective lattice, respectively. This is assured by the operators $(1 - n_{\vec{r}_j,c})$ and $n_{\vec{r}_j,c}$ in their expressions provided in that equation, which play the role of projectors onto the η-spin and spin effective lattice, respectively.

The spin-singlet two-spinon composite local $s1$ fermions of the description of Ref.[12] live on their own $s1$ effective lattice. One occupied site of such a $s1$ effective lattice involves two sites of the spin effective lattice. Consistently, for spin density $m = 0$ and spin $S_s = 0$ states of the one- and two-electron subspace considered below the number of sites of the $s1$ effective lattice reads $N_{a_{s1}}^2 = N_{a_s}^2/2 = S_c$. As justified in Refs.[12,31], for $N_a^2 \rightarrow \infty$ both the spin and $s1$ effective lattices are square lattices with spacing a_s and a_{s1}, respectively, related as $a_{s1}\sqrt{2}\, a_s$. Some further basic information on the general description introduced in Ref.[12] needed for the studies of this paper is provided in Appendix A.

E. The goals and organization of this paper

Our general aim is to show that in the one- and two-electron subspace considered below the physics of the Hubbard model on the square lattice simplifies and refers to the square-lattice quantum liquid further studied in Ref.[19]. The set of energy eigenstates that span such a subspace are generated by momentum occupancy configurations of the c and $s1$ fermions. Evidence that such a subspace is associated with nearly the whole spectral weight generated by applying one- and two-electron operators onto $m = 0$ and $x \geq 0$ ground states is provided. It is based on the relative amount of such a weight generated by application onto these states of c and $\alpha\nu$ fermion operators. The ground-state configurations of such objects were studied in Ref.[12]. Although part of our results are argued on phenomenological grounds, they emerge naturally from the scenario provided by the interplay of symmetry and the suitable quantum-object operator description used in this paper. It is found that for the Hubbard model on the square lattice in the one- and two-electron subspace only the c and $s1$ fermions play an active role. Hence one may neglect the remaining $\alpha\nu$ fermion branches considered in Ref.[12]. The states of such a subspace may have none or one spin-neutral four-spinon $s2$ fermion but such an object has vanishing momentum and vanishing energy. In Ref.[19] important physical quantities of the square-lattice quantum liquid introduced here are expressed in terms of c and $s1$ fermion energy dispersions and velocities. It is confirmed in Sections II-A and II-B that for simple one- and two-electron operators $\hat{O}$ the leading operator term $\tilde{O}$ on the right-hand side of Eq. (4) generates nearly the whole spectral weight. For such operators the terms of the general expression (4) containing commutators involving the related operator $\hat{S} = \tilde{S}$ are found to generate very little spectral weight. Hence one can reach a quite faithful representation of such operators by expressing them in terms of the c and $s1$ fermion operators.

In this paper strong evidence is found that provided that in the thermodynamic limit $N_a^2 \rightarrow \infty$ a long-range antiferromagnetic order occurs in the ground state of the related isotropic spin-1/2 Heisenberg model on the square

lattice, a similar long range order sets in in that limit in the ground state of the half-filled Hubbard model on the square lattice for $U/4t > 0$. However, it is not among our goals providing a mathematical proof that in the thermodynamic limit $N_a^2 \rightarrow \infty$, $x = 0$, $m = 0$, and vanishing temperature $T = 0$ such a long-range antiferromagnetic order sets in. Although there is no such a proof, there is a large consensus that it should be so in both the isotropic spin-1/2 Heisenberg model on the square lattice[23–25] and in the half-filled Hubbard on the square lattice[11,26–30]. One of our aims is though providing useful physical information on how the occurrence of a long-range antiferromagnetic order and a short-range spin order at $x = 0$ and $x > 0$, respectively, in the thermodynamic limit $N_a^2 \rightarrow \infty$, $m = 0$, and vanishing temperature $T = 0$ is related to the properties of the spin effective lattice. Indeed, one of our goals is to show that within the operator description used in this paper the study of the effects of hole doping on the spin subsystem simplifies. That simplification follows from the independence that the state representations of the spin $SU(2)$ symmetry, η-spin $SU(2)$ symmetry, and hidden $U(1)$ symmetry recently found in Ref.[4], respectively, have within the present description. Such state representations correspond to independent occupancy configurations of the spin-1/2 spinons in the spin effective lattice, η-spin-1/2 η-spinons in the η-spin effective lattice, and c fermions in the c effective lattice, respectively. Specifically, at $m = 0$ spin density one of the main effects of hole doping is on the number $M_s = 2S_c$ of sites of the spin effective lattice, which at $x = 0$ and $x > 0$ hole concentrations equals and differs from that of the original lattice, respectively. (We recall that for $x > 0$ the spin effective lattice is well defined only for $N_a^2 \gg 1$ very large or infinite[12].)

The microscopic processes corresponding to the effective transfer integrals $t' = t'(U/4t)$ and $t'' = t''(U/4t)$ of the Hamiltonian (5) expressed in terms of creation and annihilation rotated-electron operators are needed to characterize the type of order of the square-lattice quantum liquid. This holds for instance concerning the short-range incomensurate-spiral spin order considered in Section III-C. The qualitative changes occurring in the spin effective lattice due to hole doping are behind processes that destroy long-range antiferromagnetic order not being active and being active at $x = 0$ and for $x > 0$, respectively. In this paper strong evidence is provided that for $0 < x \ll 1$ the ground state has a short-range incomensurate-spiral spin order. The related investigations of Ref.[19] provide evidence that a spin short-range order exists for $0 < x < x_*$, whereas for $x > x_*$ the ground state is a spin disordered state without short-range spin order. Here x_* is a critical hole concentration whose magnitude is for approximately $U/4t > 1.3$ an increasing function of $U/4t$. For the intermediate $U/4t$ values of interest for the square-lattice quantum liquid studies of that reference it reads $x_* = 0.23$ for $U/4t \approx 1.3$ and $x_* = 0.28$ for $U/4t \approx 1.6$.

Another goal of this paper is defining the symmetry of the $m = 0$ and $x = 0$ ground state after its symmetry is spontaneously broken in the limit $N_a^2 \rightarrow \infty$, upon the emergence of the long-range antiferromagnetic order. It is found that at $x = 0$, $m = 0$, and vanishing temperature $T = 0$ that state symmetry is broken from $SO(3) \times SO(3) \times U(1)$ for $N_a^2 \gg 1$ large but finite to $[U(2) \times U(1)]/Z_2^2 \equiv [SO(3) \times U(1) \times U(1)]/Z_2$ for $N_a^2 \rightarrow \infty$. Finally, the $U/4t$ dependence of the energy order parameters of the $x = 0$ antiferromagnetic order and $0 < x \ll 1$ short-range incomensurate-spiral spin order are issues also addressed in this paper.

The paper is organized as follows. The introduction and basic information on the general operator description introduced in Ref.[12] is given in Section I. In Section II a suitable one- and two-electron subspace is considered. The form that the spin and $s1$ effective lattices have in it as well as the corresponding elementary excitations are issues also addressed in that section. In Section III it is shown that for $N_a^2 \rightarrow \infty$ our results are consistent with a Mott-Hubbard insulating ground state with long-range antiferromagnetic order at half filling and a ground state with short-range spin order for a well-defined range of finite hole concentrations. Strong evidence is given that for $0 < x \ll 1$ and intermediate and large values of $U/4t$ the short-range spin order has an incommensurate-spiral character. The $U/4t$ dependence of the energy order parameters is also addressed. Finally, Section III contains the concluding remarks.

II. THE SQUARE-LATTICE QUANTUM LIQUID: A TWO-COMPONENT FLUID OF CHARGE c FERMIONS AND SPIN-NEUTRAL TWO-SPINON $s1$ FERMIONS

In this section we consider a suitable one- and two-electron subspace and study the form that the spin and $s1$ effective lattices have in it. To achieve our goals, in the following we address the problem of the generation of the one- and two-electron spectral weight in terms of processes of c fermions and spinons. The picture that emerges is that of a two-component quantum liquid of charge c fermions and spin neutral two-spinon $s1$ fermions. It refers to the square-lattice quantum liquid introduced in this paper.

A. The one- and two-electron subspace

Let $|\Psi_{GS}\rangle$ be the exact ground state for $x \geq 0$ and $m = 0$ and $\hat{O}$ denote an one- or two-electron operator. Then the state,

$$\hat{O}|\Psi_{GS}\rangle = \sum_j C_j |\Psi_j\rangle \, ; \quad C_j = \langle \Psi_j | \hat{O} | \Psi_{GS}\rangle \, , \tag{11}$$

generated by application of $\hat{O}$ onto that ground state is contained in the general one- and two-electron subspace. This is the subspace spanned by the set of energy eigenstates $|\Psi_j\rangle$ such that the corresponding coefficients C_j are not vanishing. Such a subspace must contain all excitations $\hat{O}|\Psi_{GS}\rangle$ with the operator $\hat{O}$ being any of a well defined set of operators. It includes the creation and annihilation electron operator and the whole set of simple two-electron operators. For $x \geq 0$ and $m = 0$ the c and $s1$ fermion occupancies of the ground states $|\Psi_{GS}\rangle$ are found in Ref.[12].

Our goal here is finding what occupancy configurations of the objects of the description of such a reference generate a set of excited energy eigenstates $\{|\Psi_j\rangle\}$ such that $\sum_j |C_j|^2 \approx 1$ for $\hat{O}$ being a creation and annihilation electron operator and all simple two-electron operators. That set of states must contain nearly the whole spectral weight of the above one- and two-electron excitations. Their general form is provided below in Section II-E. It refers to a particular case of the momentum eigenstates considered in Ref.[12], which in general are not energy eigenstates. Fortunately, the set of such states that span the one- and two-electron subspace are found to be energy eigenstates. For an initial $x > 0$ (and $x = 0$) and $m = 0$ ground state $|\Psi_{GS}\rangle$ evidence is provided in the following that such states have excitation energy $\omega < 2\mu$ (and $\omega < \mu^0$). The inequality $\omega < 2\mu$ applies to some range of finite hole concentrations $x > 0$ and spin density $m = 0$. In turn, for the $\mu = 0$ and $m = 0$ absolute ground state with the chemical-potential zero level at the middle of the Mott-Hubbard gap the smallest energy required for creation of either one rotated-electron doubly occupied site or one rotated-hole doubly occupied site is instead given by the energy scale μ^0. This justifies why for such initial ground state the above inequality $\omega < 2\mu$ is replaced by $\omega < \mu^0$.

From the use of the invariance under the electron - rotated-electron unitary transformation of the independent $\pm 1/2$ spinons[12], one finds that the number $L_s = [L_{s,-1/2} + L_{s,+1/2}] = 2S_s$ of Eq. (10) for $\alpha = s$ of such objects generated by application of $\mathcal{N}$-electron operators onto a ground state is exactly restricted to the following range,

$$L_s = [L_{s,\,-1/2} + L_{s,\,+1/2}] = 2S_s = 0, 1, 2, ..., \mathcal{N} \, . \tag{12}$$

It follows that for the one- and two-electron subspace only the values $L_s = [L_{s,\,-1/2} + L_{s,\,+1/2}] = 2S_s = 0, 1, 2$ are allowed. Such a restriction is exact for both the model on the square and 1D lattices, as well as for any other bipartite lattice.

For a finite number $\nu \geq 2$ of spinon pairs the $s\nu$ fermions created onto a $x \geq 0$ and $m = 0$ ground state have vanishing energy and momentum[12]. A vanishing spin density $m = 0$ refers to a vanishing magnetic field $H = 0$. Hence such objects obey the criterion $\epsilon_{s\nu} = 2\nu\mu_B \, H = 0$ of Eq. (A10) of Appendix A, so that they are invariant under the electron - rotated-electron unitary transformation. Therefore, for $U/4t > 0$ they correspond to the same occupancy configurations in terms of both rotated electrons and electrons. That reveals that such $s\nu$ fermions describe the spin degrees of freedom of a number $2\nu = 4, 6, ..., 2C_s$ of electrons. It follows that nearly the whole spectral weight generated by application onto a $x \geq 0$ and $m = 0$ ground state of $\mathcal{N}$-electron operators refers to a subspace spanned by energy eigenstates with numbers in the following range,

$$[L_{s,\,-1/2} + L_{s,\,+1/2} + 2C_s - 2B_s] = 0, 1, 2, ..., \mathcal{N} \, ; \quad C_s = \sum_{\nu=1}^{C_s} \nu \, N_{s\nu} \, ; \quad B_s = \sum_{\nu=1}^{C_s} N_{s\nu} \, . \tag{13}$$

Note that owing to the above invariance of the $s\nu$ fermions with $\nu \geq 2$ spinon pairs, provided that $\mathcal{N}/N_a^2 \rightarrow 0$ and $B_s/N_a^2 \rightarrow 0$ for $N_a^2 \rightarrow \infty$ the number $B_s = \sum_\nu N_{s\nu}$ is a good quantum number. (This is a generalization of the subspace (A) defined in Ref.[12].) Consistently, the $x > 0$ (and $x = 0$ and $\mu = 0$) and $m = 0$ ground state and the set of excited states of energy $\omega < 2\mu$ (and $\omega < \mu^0$) that span the one- and two-electron subspace considered here have no $-1/2$ η-spinons, $\eta\nu$ fermions, and $s\nu'$ fermions with $\nu' \geq 3$ spinon pairs so that $N_{\eta\nu} = 0$ and $N_{s\nu'} = 0$ for $\nu' \geq 3$. Summation over the set of states that span such a subspace gives indeed $\sum_j |C_j|^2 \approx 1$ for the coefficients of the one- or two-electron excitation $\hat{O}|\Psi_{GS}\rangle$ of Eq. (11). This holds for $\hat{O}$ being the electron creation or annihilation operator or any of the simple two-electron operators. Consistently, there is both for the model on the 1D and square lattices an extremely small weight corresponding mostly to states with $N_{s3} = 1$, which is neglected within the use of the one- and two-electron subspace considered here. (Note that while the number restrictions of Eq. (12) are exact, those of Eq. (13) are a very good approximation. This is why $\sum_j |C_j|^2 \approx 1$ rather than $\sum_j |C_j|^2 = 1$ for the j summation running over the set of $\mathcal{N} = 1, 2$ states that span the one- and two-electron subspace as defined here.)

numbers	charge	+1↑el.	-1↓el.	+1↓el.	-1↑el.	singl.spin	tripl.spin	tripl.spin	tripl.spin	±2↑↓el.	+2↑el.	-2↓el.	+2↓el.	-2↑el.
δN_c^h	0	-1	1	-1	1	0	0	0	0	∓ 2	-2	2	-2	2
N_{s1}^h	0	1	1	1	1	2	2	2	2	0	2	2	2	2
$\delta N_\uparrow$	0	1	0	0	-1	0	1	-1	0	± 1	2	0	0	-2
$\delta N_\downarrow$	0	0	-1	1	0	0	-1	1	0	± 1	0	-2	2	0
$L_{s,\,+1/2}$	0	1	1	0	0	0	2	0	1	0	2	2	0	0
$L_{s,\,-1/2}$	0	0	0	1	1	0	0	2	1	0	0	0	2	2
N_{s2}	0	0	0	0	0	1	0	0	0	0	0	0	0	0
S_s	0	1/2	1/2	1/2	1/2	0	1	1	1	0	1	1	1	1
δS_c	0	1/2	$-1/2$	1/2	$-1/2$	0	0	0	0	± 1	1	-1	1	-1
δN_{s1}	0	0	-1	0	-1	-2	-1	-1	-1	± 1	0	-2	0	-2
$\delta N_{a_{s1}}$	0	1	0	1	0	0	1	1	1	± 1	2	0	2	0

TABLE I: The deviations $\delta N_c^h = -2\delta S_c$ and numbers $N_{s1}^h = [2S_s + 2N_{s2}]$ of Eq. (16) for the fourteen classes of one- and two-electron excited states of the $x > 0$ and $m = 0$ ground state that span the one- and two-electron subspace considered in this paper, corresponding electron number deviations $\delta N_\uparrow$ and $\delta N_\downarrow$, and independent-spinon numbers $L_{s,\,+1/2}$ and $L_{s,\,-1/2}$ and $s2$ fermion numbers N_{s2} restricted to the values provided in Eq. (14). The spin S_s and deviations δS_c, $\delta N_{s1} = [\delta S_c - S_s - 2N_{s2}]$, and $\delta N_{a_{s1}} = [\delta S_c + S_s]$ of each excitation are also provided.

Thus, according to Eq. (13) the numbers of independent $\pm 1/2$ spinons and that of $s2$ fermions of the excited states that span such a subspace are restricted to the following ranges,

$$\begin{aligned} L_{s,\,\pm 1/2} &= 0, 1\,; \quad N_{s2} = 0\,, \quad \text{for} \;\; \mathcal{N} = 1\,, \\ 2S_s + 2N_{s2} &= [L_{s,\,-1/2} + L_{s,\,+1/2} + 2N_{s2}] = 0, 1, 2\,, \quad \text{for} \;\; \mathcal{N} = 2\,. \end{aligned} \tag{14}$$

Here $\mathcal{N} = 1, 2$ refers to any of the $\mathcal{N}$-electron operators $\hat{O}$ whose application onto the ground state $|\Psi_{GS}\rangle$ generates the above excited states, as given in Eq. (11). Furthermore, the number of c fermions and the number of $s1$ fermions read $N_c = N = (1-x)\,N_a^2$ and $N_{s1} = [N/2 - 2N_{s2} - S_s] = (1-x)\,N_a^2/2 - [2N_{s2} + S_s]$, respectively. If in addition we restrict our considerations to the LWS-subspace of the one- and two-electron subspace[12], then $L_{s,\,-1/2} = 0$ in Eq. (14), whereas the values $L_{s,\,+1/2} = 0, 1$ for $N_{s2} = 0$ and $\mathcal{N} = 1$ remain valid and in $[2S_s + 2N_{s2}] = 0, 1, 2$ one has that $2S_s = L_{s,\,+1/2}$ for $\mathcal{N} = 2$.

As shown in Ref.[12], the numbers of independent η-spinons ($\alpha = \eta$) and independent spinons ($\alpha = s$) $L_{\alpha,\,\pm 1/2}$, the total numbers of η-spinons ($\alpha = \eta$) and spinons ($\alpha = s$) $M_{\alpha,\,\pm 1/2} = [L_{\alpha,\,\pm 1/2} + C_\alpha]$, the number of sites of the spin effective lattice $N_{a_s}^2 = 2S_c$, the number of sites of the η-spin effective lattice $N_{a_\eta}^2 = [N_a^2 - 2S_c]$, the number of c fermions $N_c = 2S_c$, and the number of c fermion holes $N_c^h = [N_a^2 - 2S_c]$ are good quantum numbers of the Hubbard model on the square lattice. The good news is that in the one- and two-electron subspace considered here the numbers $N_{a_{s1}}^2$, N_{s1}, N_{s1}^h, and N_{s2} are also good quantum numbers of such a model. The number of sites, unoccupied sites, and occupied sites of the c and $s1$ effective lattices equal those of discrete momentum values, unfilled momentum values, and filled momentum values of the c and $s1$ bands, respectively. From straightforward manipulations of Eqs. (A4) and (A5) of Appendix A for $\alpha\nu = s1$ we find that the number $N_{a_{s1}}^2 = [N_{s1} + N_{s1}^h]$ of $s1$ effective lattice sites and thus of $s1$ band discrete momentum values is in general given by,

$$N_{a_{s1}}^2 = [S_c + S_s + \sum_{\nu=3}^{C_s} (\nu - 2) N_{s\nu}]\,. \tag{15}$$

Hence for the one- and two-electron subspace considered in this paper for which $N_{s\nu} = 0$ for $\nu \geq 3$ one has that $N_{a_{s1}}^2 = [S_c + S_s]$ is a good quantum number. Consistently, for spin $S_s = 0$ that subspace is a subspace (A) as defined in Ref.[12]. It follows that $N_{s1} = [S_c - 2N_{s2}]$, $N_{s1}^h = 2N_{s2}$, and N_{s2} and hence $N_{a_{s1}}^2 = [N_{s1} + N_{s1}^h] = S_c$ are good quantum numbers. Furthermore, for the remaining spin values $S_s = 1/2$ and $S_s = 1$ such a subspace is a subspace (B) as defined in that reference. Hence $N_{s1} = [S_c - S_s]$, $N_{s1}^h = 2S_s$, and $N_{a_{s1}}^2 = [S_c + S_s]$ are good quantum numbers. It then follows from the general properties of the operator description of Ref.[12] that for the Hubbard model on the square lattice in the one- and two-electron subspace the $s1$ fermion band microscopic momenta $\vec{q}$ are good quantum numbers as well.

Moreover, use of the general expressions of $s1$ band discrete momentum values and number $N_{s1}^h = [N_{a_{s1}}^2 - N_{s1}]$ of $s1$ band unfilled momentum values with $N_{a_{s1}}^2$ given in Eq. (15) together with the restrictions in the values of the numbers of Eqs. (12), (13), and (14) and the exact result proved in Ref.[12] that one-electron (and two-electron) excitations have no overlap with excited states with none and two (and one) $s1$ band holes (and hole) reveals that

nearly the whole one- and two-electron spectral weight is contained in the subspace spanned by states whose deviation δN_c^h in the number of c band holes and number N_{s1}^h of $s1$ band holes are given by,

$$\begin{aligned} \delta N_c^h &= -2\delta S_c = -\delta N = 0, \mp 1, \mp 2\,, \\ N_{s1}^h &= S_c + S_s - N_{s1} = 2S_s + 2N_{s2} \\ &= \pm(\delta N_\uparrow - \delta N_\downarrow) + 2L_{s,\,\mp 1/2} + 2N_{s2} = L_{s,\,-1/2} + L_{s,\,+1/2} + 2N_{s2} = 0, 1, 2\,. \end{aligned} \quad (16)$$

Here δN is the deviation relative to the initial ground state in the number of electrons, $\delta N_\uparrow$ and $\delta N_\downarrow$ are those in the number of spin-projection $\uparrow$ and $\downarrow$ electrons, respectively, N_{s2} is the number of the excited-state $s2$ fermions, and $L_{s,\,\pm 1/2}$ is that of independent spinons of spin projection $\pm 1/2$. We emphasize that for an initial $m = 0$ and $S_s = 0$ ground state the numbers $N_{s2} = L_{s,\,\pm 1/2} = N_{s1}^h = 0$ vanish[12].

The deviations δN_c^h and numbers N_{s1}^h of Eq. (16) for the fourteen classes of one- and two-electron excited states of the $x > 0$ and $m = 0$ ground state that span the one- and two-electron subspace, corresponding electron number deviations $\delta N_\uparrow$ and $\delta N_\downarrow$, and independent-spinon numbers $L_{s,\,+1/2}$ and $L_{s,\,-1/2}$ and $s2$ fermion numbers N_{s2} restricted to the values provided in Eq. (14) are given in Table I. For $N_{s2} = 1$ spin-siglet excited states the $s2$ effective lattice has a single site and the corresponding $s2$ band a single vanishing discrete momentum value, $\vec{q} = 0$, occupied by the $s2$ fermion[12]. We recall that such a $s2$ fermion is invariant under the electron - rotated-electron unitary transformation and thus has vanishing energy, consistently with the invariance condition of Eq. (A10) of Appendix A for $\alpha\nu = s2$ and vanishing magnetic field $H = 0$.

As mentioned above, the initial $x > 0$ and $m = 0$ ground states of the one- and two-electron subspace have zero holes in the $s1$ band so that $\delta N_{s1}^h = N_{s1}^h$ for the excited states. This follows from all $M_s = 2S_c = N$ spinons being confined within the two-spinon bonds of the $N_{s1} = M_s/2$ $s1$ fermions. The one- and two-electron subspace is spanned by the states of Table I generated by creation or annihilation of $|\delta N_c^h| = 0, 1, 2$ holes in the c momentum band and $N_{s1}^h = 0, 1, 2$ holes in the $s1$ band plus small momentum and low energy particle-hole processes in the c band. The charge excitations of $x > 0$ and $m = 0$ initial ground states consist of a single particle-hole process in the c band of arbitrary momentum and energy compatible with its momentum and energy bandwidths, plus small-momentum and low-energy c fermion particle-hole processes. Such charge excitations correspond to state representations of the global $U(1)$ symmetry and refer to the type of states denoted by "charge" in the table. The one-electron spin-doublet excitations correspond to the four types of states denoted by "$\pm 1\sigma$el." in Table I where $+1$ and -1 denotes creation and annihilation, respectively, and $\sigma = \uparrow, \downarrow$. The spin-singlet and spin-triplet excitations refer to the four types of states denoted by "singl.spin" and "tripl.spin" in the table. The two-electron excitations whose electrons are in a spin-singlet configuration and those whose two created or annihilated electrons are in a spin-triplet configuration correspond to the five types of states "± 2 $\uparrow\downarrow$el." and "$\pm 2\sigma$el." of that table where $+2$ and -2 denotes creation and annihilation, respectively, of two electrons.

For the Hubbard model on the square lattice such fourteen types of states are energy eigenstates and nearly exhaust the whole one- and two-electron spectral weight. Excited states of classes other than those of the table contain nearly no one- and two-electron spectral weight. Such a weight analysis applies to the 1D Hubbard model as well. For the corresponding quantum liquid describing the Hamiltonian (1) in the one- and two-electron subspace, the numbers $2S_c$, $2S_\eta$, $2S_s$, and $-2S_s^{x_3}$ associated with the global $SO(3) \times SO(3) \times U(1)$ symmetry are given by,

$$2S_c = (1-x)\,N_a^2\,;\quad 2S_\eta = -2S_\eta^{x_3} = x\,N_a^2\,;\quad 2S_s = (1-x)\,N_a^2 - 2[N_{s1} + 2N_{s2}]\,;\quad -2S_s^{x_3} = m\,N_a^2 = 2S_s - 2L_{s,-1/2}\,. \quad (17)$$

For such a quantum liquid the number of sites of the spin effective lattice $N_{a_s}^2 = 2S_c$ and corresponding spacing a_s given in Eq. (A8) of Appendix A read,

$$N_{a_s}^2 = (1-x)\,N_a^2\,;\quad a_s = \frac{a}{\sqrt{1-x}}\,,\quad (1-x) > 1/N_a^2\,, \quad (18)$$

respectively. Its sites refer to those singly occupied by rotated electrons in the original lattice. In turn, the sites of the η-spin lattice also introduced in Ref.[12] refer to the sites doubly occupied and unoccupied by rotated electrons in the original lattice.

For the Hubbard model in the one- and two-electron subspace the concept of a η-spin lattice considered in Ref.[12] is useless. Indeed, for that subspace such a lattice either is empty ($x > 0$) or does not exist ($x = 0$). This is because the η-spin degrees of freedom of the states that span that subspace are the same as those of the $C_\eta = \sum_{\nu=1}^{C_\eta} \nu\, N_{\eta\nu} = (N_a^2/2 - S_c - S_\eta) = 0$ vacuum $|0_\eta; N_{a_\eta}^2\rangle$ of Eq. (A3) of Appendix A. For states for which $S_c = N_a^2/2$ and thus $N_{a_\eta}^2 = S_\eta = 0$ the η-spin lattice does not exist and thus the spin effective lattice is identical to the original lattice. This is argued below in Section III-C to be a necessary condition for a spontaneous symmetry breaking and emergence of a long-range antiferromagnetic order to occur in the ground state as $N_a^2 \to \infty$. In turn, for $S_c < N_a^2/2$ the η-spin

degrees of freedom correspond to a single occupancy configuration of the $N^2_{a_\eta}$ independent $+1/2$ η-spinons. Such objects are invariant under the electron - rotated-electron transformation and thus play the role of unoccupied sites of the η-spin lattice[12]. Indeed, for the one- and two-electron subspace the corresponding number of η-spin lattice occupied sites $C_\eta = \sum_{\nu=1}^{C_\eta} \nu\, N_{\eta\nu}$ vanishes. Only for states and subspaces for which $N^2_{a_\eta}/N^2_a = [1 - 2S_c/N^2_a]$ is finite and the inequality $0 < C_\eta < N^2_{a_\eta}$ holds is the concept of a η-spin effective lattice useful. For a given state, $C_\eta + C_s$ is the number of sites of the original lattice whose electron occupancy configurations are not invariant under the electron - rotated-electron unitary transformation. For the states that span the one- and two-electron subspace the numbers C_η and C_s are given by $C_\eta = 0$ and $C_s = [N_{s1} + 2N_{s2}]$, respectively. For $x = 0$ (and $x = 1$) one finds $N^2_{a_\eta} = 0$ and $N^2_{a_s} = N^2_a$ (and $N^2_{a_\eta} = N^2_a$ and $N^2_{a_s} = 0$), so that there is no η-spin (and no spin) effective lattice and the spin (and η-spin) effective lattice equals the original lattice.

As further confirmed below, for the one- and two-electron subspace considered here only the c and $s1$ fermions play an active role. Straightforward manipulations of the general expressions given in Eq. (15) and Eqs. (A4)-(A9) of Appendix A and related expressions provided in Ref.[12] reveal that for that subspace the number $N^2_{a_{s1}}$ of $s1$ band discrete momentum values, N_{s1} of $s1$ fermions, and N^h_{s1} of $s1$ fermion holes are given by,

$$N^2_{a_{s1}} = [N_{s1} + N^h_{s1}] = [S_c + S_s]\,; \quad N_{s1} = [S_c - S_s - 2N_{s2}]\,; \quad N^h_{s1} = [2S_s + 2N_{s2}] = 0, 1, 2\,, \tag{19}$$

respectively. In turn, the corresponding c effective lattice, c momentum band, and c fermion numbers read,

$$N^2_{a_c} = [N_c + N^h_c] = N^2_a\,; \quad N_c = 2S_c = (1 - x)\, N^2_a\,; \quad N^h_c = x\, N^2_a\,. \tag{20}$$

B. Confirmation for 1D that most one-electron spectral weight is generated by processes obeying the ranges of Eqs. (13), (14), and (16)

Above the transformation laws under the electron - rotated-electron transformation of the $\alpha\nu$ fermions were used to show that nearly the whole spectral weight of the one- and two-electron excitations of the Hubbard model on the square lattice is generated by processes obeying the ranges of Eqs. (13), (14), and (16). Similar results apply to the 1D model.

The terms of one- or two-electron operators $\hat{O}$ on the right-hand side of the first equation of (4) that generate the excitations $\hat{O}|\Psi_{GS}\rangle$ of Eq. (11) may be expressed in terms of the of c fermion operators, spinon operators, and η-spinon operators given in Eqs. (6)-(9). This is done by use of the operator relations provided in Eq. (A1) of Appendix A. Concerning the contributions to the $\hat{O}$ expression provided in Eq. (4) containing commutators involving the operator $\tilde{S} = -(t/U)\,[\tilde{T}_{+1} - \tilde{T}_{-1}] + \mathcal{O}(t^2/U^2)$, to fulfill such a task one takes into account that independently of their form, the additional operator terms $\mathcal{O}(t^2/U^2)$ of higher order are products of the kinetic operators $\tilde{T}_0$, $\tilde{T}_{+1}$, and $\tilde{T}_{-1}$ of Eq. (2).

From such an analysis one finds that the elementary processes associated with the one- and two-electron subspace number value ranges of Eqs. (13), (14), and (16) are fully generated by the leading-order operator $\tilde{O}$. In turn, the processes generated by the operator terms containing commutators involving the operator $\tilde{S}$ refer to excitations whose number value ranges are different from those of Eqs. (13), (14), and (16). This confirms that such processes generate very little one- and two-electron spectral weight, consistently with the exact number restrictions of Eq. (12), the approximate number restrictions of Eq. (13), and the results of Ref.[12].

For the Hubbard model on the 1D lattice also often considered in the studies of that reference, the spectral-weight distributions can be calculated explicitly by the pseudofermion dynamical theory associated with the model exact solution, exact diagonalization of small chains, and other methods. From the use of the same arguments as for the model on the square lattice one finds that at 1D the one- and two-electron subspace considered in this paper corresponds to the same number deviations and numbers as for the square lattice. In addition, the relative one-electron spectral weight generated by different types of microscopic processes can be studied by means of the above methods. That program is fulfilled in Ref.[32]. The results of that reference confirm the dominance of the processes associated with the number value ranges provided in Eqs. (14) and (16). They refer spacifically to operators $\hat{O}$ and $\tilde{O}$ that are electron and rotated-electron, respectively, creation or annihilation operators. Such studies confirm that the operator $\tilde{O}$ generates *all* processes associated with the number value ranges of Eqs. (14) and (16) and number values of Table I. In addition, it also generates some of the non-dominant processes. That is confirmed by the weights given in Table 1 of Ref.[32], which correspond to the dominant processes associated with only these ranges. The small missing weight refers to excitations whose number value ranges are not those of Eqs. (14) and (16) but whose weight is also generated by the operator $\tilde{O}$. Indeed, that table refers to $U/4t \rightarrow \infty$ so that $\hat{O} = \tilde{O}$ and the operator terms of the $\hat{O}$ expression provided in Eq. (4) containing commutators involving the operator $\tilde{S}$ vanish.

On the other hand, for finite values of $U/4t$ all dominant processes associated with the number value ranges of Eqs. (14) and (16) and number values provided in Table I are generated by the operator $\tilde{O}$. In turn, the small spectral weight associated with excitations whose number value ranges are different from those are generated both by that operator and the operator terms of the $\hat{O}$ expression of Eq. (4) containing commutators involving the operator $\tilde{S}$. For the model on the 1D lattice the small one-electron spectral weight generated by the non-dominant processes is largest at half filling and $U/4t \approx 1$.

For $x \geq 0$ the one- and two-electron subspace is spanned by states with vanishing rotated-electron double occupancy. This holds both for the Hubbard model on the 1D and square lattices. Generalization of the results to the range $x \leq 0$ reveals that then such a subspace is spanned by states with vanishing rotated-hole double occupancy. That property combined with the particle-hole symmetry explicit at $x = 0$ and $\mu = 0$, implies that the relative spectral-weight contributions from different types of one-electron addition excitations given in Fig. 2 of Ref.[32] for the 1D model at half filling leads to similar corresponding relative weights for half-filling one-electron removal. Analysis of that figure confirms that for the corresponding one-electron removal spectrum the dominant processes associated with the number value ranges of Eqs. (14) and (16) and number values given in Table I refer to the states called in figure 1 holon - 1 $s1$ hole states. Their minimum relative weight of about 0.95 is reached at $U/4t \approx 1$. For other hole concentrations $x > 0$ and values of $U/4t$ the relative weight of such states is always larger than 0.95, as confirmed from analysis of Figs. 1 and 2 and Table 1 of Ref.[32].

For the Hubbard model on the square lattice the explicit derivation of one- and two-electron spectral weights is a more involved problem. The number value ranges of Eqs. (13), (14), and (16) and number values provided in Table I for the one- and two-electron subspace also apply, implying similar results for the relative spectral weights of one- and two-electron excitations. Consistently and as mentioned above, there is an exact selection rule valid both for the Hubbard model on a 1D and square lattices that confirms that $N^h_{s1} = 1$ and $N^h_{s1} = 0, 2$ for one-electron excitations and two-electron excitations, respectively. It follows from the expression provided in Eq. (A7) of Appendix A for the quantum number $P^h_{s1} = e^{i\pi N^h_{s1}} = e^{i\pi N} = \pm 1$. It reveals that for $\delta N = \pm 1$ (and $\delta N = \pm 0$ and $\delta N = \pm 2$) excited states the number N^h_{s1} of holes in the $s1$ band must be always an odd (and even) integer. Here δN is the deviation in the electron number N under a transition from a $x > 0$ and $m = 0$ ground state to such excited states. This implies that one-electron (and two-electron) excitations do not couple to excited states with two holes (and one hole) in the $s1$ band. Indeed, for such excitations one has that $e^{i\pi\delta N} = -1$ (and $e^{i\pi\delta N} = +1$), so that $e^{i\pi\delta N^h_{s1}} = -1$ (and $e^{i\pi\delta N^h_{s1}} = +1$).

C. The spin and $s1$ effective lattices for the one- and two-electron subspace

According to the restrictions and numbers values of Eqs. (14) and (16) and Table I, the states that span the one- and two-electron subspace may involve none or one $s2$ fermion. As confirmed in Ref.[19], it is convenient to express the one- and two-electron excitation spectrum relative to initial $x > 0$ and $m = 0$ ground states in terms of the deviations in the numbers of c effective lattice and $s1$ effective lattice unoccupied sites. Those are given explicitly in Eq. (16) and Table I. Note that the number of $s1$ fermions provided in Eq. (19) can be written as $N_{s1} = [(1-x)N^2_a/2 - S_s - 2N_{s2}]$ where $S_s = 0$ for $N_{s2} = 1$ and $S_s = 0, 1/2, 1$ for $N_{s2} = 0$.

As discussed above, for $N_{s2} = 1$ spin-singlet excited energy eigenstates the single $s2$ fermion has vanishing energy and momentum and consistently with Eq. (A10) of Appendix A, for vanishing magnetic field $H = 0$ it is invariant under the electron - rotated-electron unitary transformation. Therefore, the only effect of its creation and annihilation is in the numbers of occupied and unoccupied sites of the $s1$ effective lattice. Its creation can then be accounted for merely by small changes in the occupancies of the discrete momentum values of the $s1$ band, as discussed below. Hence the only composite object whose internal occupancy configurations in the spin effective lattice are important for the physics of the Hamiltonian (1) in the one- and two-electron subspace is the spin-neutral two-spinon $s1$ fermion and related spin-singlet two-spinon $s1$ bond particle[12,31].

It is confirmed below that for the Hubbard model in the one- and two-electron subspace and alike for the $s2$ fermion, the presence of independent spinons is felt through the numbers of occupied and unoccupied sites of the $s1$ effective lattice. In turn, the number of independent $+1/2$ η-spinons equals that of the unoccupied sites of the c effective lattice. Therefore, when acting onto that subspace, the Hubbard model refers to a two-component quantum liquid that can be described only in terms of c fermions and $s1$ fermions.

For $x > 0$ and states belonging to the one- and two-electron subspace the spin effective lattice has a number of sites $N^2_{a_s} = (1-x)\, N^2_a$. Its value is smaller than that of the original lattice. The lattice constant a_s provided in Eq. (A8) of Appendix A for $\alpha = s$ reads $a_s \approx a/\sqrt{1-x}$ for such states, as given in Eq. (18). It is such that the area L^2 of the system is preserved. Any real-space point within the spin effective lattice corresponds to the same real-space point in the system original lattice. Except for a suitable phase factor, a local $s1$ fermion has the same internal structure

as the corresponding $s1$ bond-particle[12,19]. The $s1$ fermion spinon occupancy configurations considered in Ref.[31] are expected to be a good approximation provided that the ratio $N_{a_s}^2/N_a^2$ and thus the electronic density $n = (1-x)$ are finite in the limit $N_a^2 \to \infty$. This is met for the hole concentration range $x \in (0, x_*)$ where $x_* < 1$ for which according to the studies of Ref.[19] the maximum magnitude of the $s1$ fermion spinon pairing energy is finite.

Within the $N_a^2 \gg 1$ limit that the description used in the studies of this paper refers to, there is for the states that span the one- and two-electron subspace commensurability between the real-space distributions of the $N_{a_{s1}}^2 \approx N_{s1}$ sites of the $s1$ effective lattice and the $N_{a_s}^2 \approx 2N_{s1}$ sites of the spin effective lattice. For $(1-x) \geq 1/N_a^2$ and $N_a^2 \gg 1$ the spin effective lattice has $N_{a_s}^2 = (1-x)\,N_a^2$ sites and from the use of the expression given in Eq. (19) for the number of $s1$ effective lattice sites $N_{a_{s1}}^2$ and Eq. (A9) of Appendix A for the corresponding spacing a_{s1} we find,

$$a_{s1} = a_s \sqrt{\frac{2}{1+\frac{2S_s}{(1-x)N_a^2}}} \approx \sqrt{2}\,a_s \left(1 - \frac{2S_s}{2(1-x)}\frac{1}{N_a^2}\right) \approx \sqrt{2}\,a_s\,, \quad S_s = 0, \frac{1}{2}, 1\,. \tag{21}$$

For $N_{s1}^h = 0$ states such as the $x \geq 0$ and $m = 0$ ground states the square spin effective lattice has two well-defined sub-lattices, which we call sub-lattice A and B, respectively. As discussed in Ref.[31], for $N_{s1}^h = 1, 2$ states the spin effective lattice has two bipartite lattices as well, with one or two extra sites corresponding to suitable boundary conditions. The two spin effective sub-lattices have spacing $a_{s1} = \sqrt{2}\,a_s$. The fundamental translation vectors of the sub-lattices A and B read,

$$\vec{a}_{s1} = \frac{a_{s1}}{\sqrt{2}}(\vec{e}_{x_1} + \vec{e}_{x_2})\,, \quad \vec{b}_{s1} = -\frac{a_{s1}}{\sqrt{2}}(\vec{e}_{x_1} - \vec{e}_{x_2})\,, \tag{22}$$

respectively. Here $\vec{e}_{x_1}$ and $\vec{e}_{x_2}$ are the unit vectors and x_1 and x_2 Cartesian coordinates. As confirmed in Ref.[31], the vectors given in Eq. (22) are the fundamental translation vectors of the $s1$ effective lattice.

In the case of $x \geq 0$, $m = 0$, and $N_{s1}^h = 0$ ground states whose $s1$ momentum band is full and all $N_{a_{s1}}^2$ sites of the $s1$ effective lattice are occupied we consider that the square root N_{a_s} of the number $N_{a_s}^2$ of sites of the spin effective lattice is an integer. It then follows that the spin effective lattice is a square lattice with $N_{a_s} \times N_{a_s}$ sites. Thus the square root $N_{a_{s1}}$ of the number $N_{a_{s1}}^2$ of sites of the $s1$ effective lattice cannot in general be an integer number yet $N_{a_{s1}}^2$ is. However, within the $N_a^2 \gg 1$ limit considered here we use the notation $N_{a_{s1}}^2$ for the number of sites of the $s1$ effective lattice.

D. The quantum liquid of c fermions and $s1$ fermions: Why only such objects play an active role?

For the one- and two-electron subspace considered in this paper the number $N_{a_{s1}}^2$ of sites of the $s1$ effective lattice and $s1$ band discrete momentum values, N_{s1} of $s1$ fermions, and N_{s1}^h of $s1$ fermion holes have expressions given in Eq. (19). The corresponding numbers of the c effective lattice and c band are provided in Eq. (20). For that subspace the $s1$ band is either full and thus is filled by $N_{s1} = N_{a_{s1}}^2 = 2S_c = N_{a_s}^2$ $s1$ fermions or has one or two holes. Furthermore, one-electron and two-electron excitations have no overlap with excited states with two holes and one hole in the $s1$ band, respectively. Specifically, excited states with a single hole in the $s1$ band correspond to one-electron excitations and those with $N_{s1}^h = 0, 2$ holes in that band refer to two-electron excitations, as given in Table I. Excited states with $N_{s1}^h = 3$ (and $N_{s1}^h = 4$) holes in the $s1$ momentum band correspond to very little one-electron (and two-electron) spectral weight and are ignored within the use of the one- and two-electron subspace considered here.

We now justify why the square-lattice quantum liquid corresponding to the Hubbard model on the square lattice in the one- and two-electron subspace may be described only by c and $s1$ fermions on their c and $s1$ effective lattices, respectively. According to the number value ranges of Eqs. (14) and (16) and number values provided in Table I, the one- and two-electron subspace is spanned by excited states having either none $N_{s2} = 0$ or one $N_{s2} = 1$ spin-neutral four-spinon $s2$ fermion. $N_{s2} = 1$ spin-singlet excited states have no independent spinons. One then finds from the use of Eq. (A5) of Appendix A for $\alpha\nu = s2$ that $N_{s2}^h = 0$ so that such states have no holes in the $s1$ momentum band and thus $N_{a_{s2}}^2 = 1$. This means that for such states the $s2$ fermion occupies a $s2$ band with a single vanishing momentum value. Since the $s2$ fermion under consideration has both vanishing momentum and energy and is invariant under the electron - rotated-electron unitary transformation, the only explicit effect of its creation is onto the numbers of occupied and unoccupied sites of the $s1$ effective lattice and corresponding numbers of $s1$ band $s1$ fermions and $s1$ fermion holes. Specifically, according to the expressions provided in Eq. (19) and number values of Table I, the deviations $\delta S_c = \delta S_s = 0$ and $\delta N_{s2} = 1$ generated by a state transition involving creation of one $s2$ fermion lead to deviations in the number of $s1$ fermions and $s1$ fermion holes given by $\delta N_{s1} = -2\delta N_{s2} = -2$ and $\delta N_{s1}^h = 2\delta N_{s2} = 2$, respectively.

Moreover, the ranges of Eqs. (14) and (16) and number values of Table I confirm that such $N_{s2} = 1$ excited states have zero spin, $S_s = 0$. According to Eq. (19), the number of holes in the $s1$ band is $N^h_{s1} = 2N_{s2} = 2$ for such states, in contrast to $N^h_{s1} = 0$ for the initial ground state. In turn, the number $N^2_{a_{s1}}$ of sites of the $s1$ effective lattice remains unaltered. Following the annihilation of two $s1$ fermions and creation of one $s2$ fermion, two unoccupied sites appear in the $s1$ effective lattice. As a result two holes emerge in the $s1$ band as well. The emergence of these unoccupied sites and holes involves two virtual processes where (i) two $s1$ fermions are annihilated and four independent spinons are created and (ii) the latter independent spinons are annihilated and the $s2$ fermion is created.

Hence the only explicit net effect of the creation of a single vanishing-energy and zero-momentum $s2$ fermion is the annihilation of two $s1$ fermions and corresponding emergence of two holes in the $s1$ band and two unoccupied sites in the $s1$ effective lattice. Therefore, in the case of the one- and two-electron subspace one can ignore that object in the theory provided that the corresponding changes in the $s1$ band and $s1$ effective lattice occupancies are accounted for. Within neutral $s1$ fermion particle-hole processes of transitions between two excited states with a single $s2$ fermion, two of the four spinons of such an object are used in the motion of $s1$ fermions around in the $s1$ effective lattice. Indeed, such two spinons play the role of unoccupied sites of that lattice[12,31], consistently with the expression $N^h_{s1} = 2N_{s2}$ given in Eq. (19) for $2S_s = 0$.

Also the $L_s = 2S_s$ independent spinons play the role of unoccupied sites of the $s1$ effective lattice. Again, this is consistent with the expression $N^h_{s1} = L_s = 2S_s = 1, 2$ provided in Eq. (19) for the number of unoccupied sites of the $s1$ effective lattice and of $s1$ fermion holes of the corresponding $N_{s2} = 0$ excited states. As given in Eqs. (14) and (16) and Table I, the one- and two-electron subspace L_s allowed values are $L_s = [L_{s\,,-1/2} + L_{s\,,+1/2}] = 2S_s = 0, 1, 2$. For $2S_s = 1, 2$ one has that $N_{s2} = 0$. Now in contrast to creation of a single $s2$ fermion, a deviation $\delta 2S_s = 1, 2$ generated by a transition from the ground state to such $2S_s = 1, 2$ excited states may lead to deviations in the numbers of occupied and unoccupied sites of the $s1$ effective lattice and corresponding $s1$ fermion and $s1$ fermion holes that do not obey the usual equality $\delta N_{s1} = -\delta N^h_{s1}$. Indeed, in the present case $2\delta S_c = \pm 1$ for $\delta N^h_{s1} = 2\delta S_s = 1$ and $2\delta S_c = 0, \pm 2$ for $\delta N^h_{s1} = 2\delta S_s = 2$. Hence according to the expressions provided in Eq. (19), such deviations lead to deviations in the numbers of occupied and unoccupied sites of the $s1$ effective lattice and corresponding numbers of $s1$ fermions and $s1$ fermion holes. Those read $\delta N_{s1} = [\delta S_c - \delta S_s]$ and $\delta N^h_{s1} = \delta 2S_s$, respectively. It follows that the total number of sites and thus of discrete momentum values of the $s1$ band may change under such transitions. This leads to an additional deviation $\delta N^2_{a_{s1}} = [\delta S_c + \delta S_s]$. As given in Table I, for one-electron excited states one has that $\delta N^h_{s1} = 2\delta S_s = 1$ and $2\delta S_c = \pm 1$. As a result, $\delta N_{s1} = \pm 1/2 - 1/2 = -1, 0$ and $\delta N^2_{a_{s1}} = \pm 1/2 + 1/2 = 0, -1$. In turn, for $N_{s2} = 0$ two-electron excited states one has $\delta N^h_{s1} = 2\delta S_s = 2$ and $2\delta S_c = 0, \pm 2$. Thus $\delta N_{s1} = -1, (\pm 1 - 1) = -2, -1, 0$ and $\delta N^2_{a_{s1}} = 1, (\pm 1 + 1) = 0, 1, 2$.

For the $s1$ fermion operators $f^\dagger_{\vec{q},s1}$ and $f_{\vec{q},s1}$, excitations that involve changes $\delta N^2_{a_{s1}} = [\delta S_c + \delta S_s]$ in the number of sites and discrete momentum values of the $s1$ effective lattice and $s1$ band, respectively, correspond to transitions between different quantum problems. Indeed, such operators act onto subspaces spanned by neutral states, which conserve S_c, S_s, and $N^2_{a_{s1}}$. In turn, the generator of a non-neutral excitation is the product of two operators. The first operator makes small changes in the $s1$ effective lattice or corresponding $s1$ momentum band. Such changes follows the above deviations $\delta N^2_{a_{s1}} = [\delta S_c + \delta S_s]$. The second operator is a $s1$ fermion operator or a product of such operators appropriate to the excited-state subspace.

Also the vanishing momentum and energy $L_{\eta,+1/2} = x\,N^2_a$ independent $+1/2$ η-spinons are invariant under the electron - rotated-electron unitary transformation. Their creation or annihilation may be accounted for by small suitable changes in occupancies of the c effective lattice and c momentum band. For $x > 0$ and the one- and two-electron subspace considered here such independent $+1/2$ η-spinons correspond to a single occupancy configuration associated with the η-spin vacuum $|0_\eta; N^2_{a_\eta}\rangle$ of Eq. (A3) of Appendix A. In turn, the degrees of freedom of the rotated-electron occupancies of such $x\,N^2_a$ sites of the original lattice associated with the $U(1)$ symmetry refer to the unoccupied sites of the c effective lattice of Eq. (20) and corresponding c band holes. Hence the number $L_{\eta,+1/2} = x\,N^2_a$ of independent $+1/2$ η-spinons equals that $N^h_c = x\,N^2_a$ of unoccupied sites of the c effective lattice and corresponding c band holes. This confirms that the deviations $\delta L_{\eta,+1/2} = (\delta x)\,N^2_a$ originated by creation and annihilation of independent $+1/2$ η-spinons within the one- and two-electron subspace has no effects on the physics other than the corresponding deviation $\delta N^h_c = (\delta x)\,N^2_a$ in the number of unoccupied sites of the c effective lattice and c band holes.

Spin-singlet excitations generated by application onto a $m = 0$ and $x \geq 0$ initial ground state of the operator $f^\dagger_{0,s2}\,f_{\vec{q},s1}\,f_{\vec{q}',s1}$ where $\vec{q}$ and $\vec{q}'$ are the momenta of the two emerging $s1$ fermion holes are neutral states which conserve S_c, S_s, and $N^2_{a_{s1}}$. (See Table I.) The implicit role of the $s2$ fermion creation operator $f^\dagger_{0,s2}$ is exactly canceling the contributions of the annihilation of the two $s1$ fermions of momenta $\vec{q}$ and $\vec{q}'$ to the commutator $[\hat{q}_{s1\,x_1}, \hat{q}_{s1\,x_2}]$ of the $s1$ translation generators in the presence of the fictitious magnetic field $\vec{B}_{s1}$ of Eq. (A2) of Appendix A. This ensures that the overall excitation is neutral. Since the $s2$ fermion has vanishing energy and momentum and the $s1$ band and its number $N^2_{a_{s1}}$ of discrete momentum values remain unaltered, one can effectively consider that the generator of

such an excitation is $f_{\vec{q},s1}\, f_{\vec{q}',s1}$ and omit the $s2$ fermion creation operator. Its only role is ensuring that the overall excitation is neutral and the two components of the $s1$ fermion microscopic momenta can be specified. It follows that for the one- and two-electron subspace the operators $f_{\vec{q},s1}\, f_{\vec{q}',s1}$, $f^{\dagger}_{\vec{q}',s1}\, f^{\dagger}_{\vec{q},s1}$, $f^{\dagger}_{\vec{q},s1}\, f_{\vec{q}',s1}$, and $f_{\vec{q},s1}\, f^{\dagger}_{\vec{q}',s1}$ generate neutral excitations.

In summary, when acting onto the one- and two-electron subspace considered in Section I-A, the Hubbard model on a square lattice refers to a two-component quantum liquid described in terms of two types of objects on the corresponding effective lattices and momentum bands: The charge c fermions and spin-neutral two-spinon $s1$ fermions. The one- and two-electron subspace can be divided into smaller subspaces that conserve S_c and S_s. Those are spanned by states of general form given below in Section II-E. When expressed in terms of c and $s1$ fermion operators, the Hubbard model on a square lattice in the one- and two-electron subspace is the square-lattice quantum liquid further studied in Ref.[19]. The presence of independent $+1/2$ spinons or of a composite $s2$ fermion is accounted for by the values of the occupied and unoccupied sites numbers of the $s1$ effective lattice and corresponding $s1$ fermion and $s1$ fermion holes. In turn, the number of independent $+1/2$ η-spinons equals that of the unoccupied sites of the c effective lattice and c band holes. Otherwise, the presence of vanishing momentum and energy independent spinons or of a single spin-neutral four-spinon $s2$ fermion as well as that of independent $+1/2$ η-spinons has no explicit direct effects on the physics. This property follows from all such objects being invariant under the electron - rotated-electron unitary transformation[12].

The quantum-liquid c fermions are η-spinless and spinless objects without internal degrees of freedom and structure whose effective lattice is identical to the original lattice. For the complete set of $U/4t > 0$ energy eigenstates that span the Hilbert space the occupied sites (and unoccupied sites) of the c effective lattice correspond to those singly occupied (and doubly occupied and unoccupied) by the rotated electrons. The corresponding c band has the same shape and momentum area as the first Brillouin zone.

In contrast, the quantum-liquid composite spin-neutral two-spinon $s1$ fermions have internal structure and the definition of the $s1$ effective lattice in terms of both the original lattice and the spin effective lattice as well as the spinon occupancy configurations that describe such objects is for the one- and two-electron subspace a more complex problem[31]. It is simplified by the property of the states that span such a subspace that the corresponding $s1$ effective lattice has none, one, or two unoccupied sites.

E. The c and $s1$ fermion momentum values and the energy eigenstates

Here we provide the specific form that the momentum energy eigenstates considered in Ref.[12] have in the one- and two-electron subspace. Such states refer to a complete set of states in the full Hilbert space. In general they are not energy eigenstates. Fortunately, in the one- and two-electron subspace such momentum energy eigenstates are as well energy eigenstates. This confirms the usefulness of the square-lattice quantum liquid that refers to that subspace.

The $s1$ band discrete momentum values $\vec{q}_j$ where $j = 1, ..., N^2_{a_{s1}}$ are the conjugate of the real-space coordinates $\vec{r}_j$ of the $s1$ effective lattice for which also $j = 1, ..., N^2_{a_{s1}}$. The same applies to the c band discrete momentum values $\vec{q}_j$ and the c effective lattice real-space coordinates $\vec{r}_j$ where in both cases $j = 1, ..., N^2_a$. (The latter lattice is identical to the original lattice.) The c translation generators $\hat{\vec{q}}_c$ commute with both the Hamiltonian and momentum operator for the whole Hilbert space[12]. This is why the c band discrete momentum values are good quantum numbers. In turn, the $s1$ translation generators $\hat{\vec{q}}_{s1}$ in the presence of the fictitious magnetic field $\vec{B}_{s1}$ of Eq. (A2) of Appendix A do not commute in general with the Hamiltonian of the Hubbard model on the square lattice. Combining the results of Ref.[12] with the specific properties of that model in the one- and two-electron subspace reveals that in the neutral subspaces of such a subspace the $s1$ translation generators $\hat{\vec{q}}_{s1}$ do commute with both the Hamiltonian and momentum operator. This is why for the present square-lattice quantum liquid the $s1$ fermion discrete momentum values $\vec{q} = [q_{x1}, q_{x2}]$ are good quantum numbers and thus are conserved. The c and $s1$ translation generators read[12],

$$\hat{\vec{q}}_c = \sum_{\vec{q}} \vec{q}\, \hat{N}_c(\vec{q})\,; \quad \hat{\vec{q}}_{s1} = \sum_{\vec{q}} \vec{q}\, \hat{N}_{s1}(\vec{q})\,. \tag{23}$$

Here $\hat{N}_c(\vec{q})$ and $\hat{N}_{s1}(\vec{q})$ are the momentum distribution-function operators,

$$\hat{N}_c(\vec{q}) = f^{\dagger}_{\vec{q},c}\, f_{\vec{q},c}\,; \quad \hat{N}_{s1}(\vec{q}) = f^{\dagger}_{\vec{q},s1}\, f_{\vec{q},s1}\,, \tag{24}$$

respectively. For the Hubbard model on the square lattice in the one- and two-electron subspace the expression of the momentum operator simplifies. It reads,

$$\hat{\vec{P}} = \hat{\vec{q}}_c + \hat{\vec{q}}_{s1}\,. \tag{25}$$

Indeed, we recall that in it the $c2$ fermion, independent $\pm 1/2$ spinons, and independent $+1/2$ η-spinons have vanishing momentum.

Since in contrast to the c fermions, the $s1$ fermions have internal structure, how is the $s1$ fermion momentum $\vec{q}$ related to the two underlying spinons? Independent spinons carry no momentum and are invariant under the electron - rotated-electron unitary transformation[12]. On the other hand, within the LWS representation of the spin $SU(2)$ algebra[12], the spin-down spinon of the spin-singlet two-spinon the $s1$ fermion of momentum $\vec{q}$ carries momentum $\vec{q}$ and its spin-up spinon carries momentum $-\vec{q}$. In turn, within the highest-weight state (HWS) representation of that algebra, its spin-down spinon carries momentum $-\vec{q}$ and its spin-up spinon carries momentum $\vec{q}$. Alike in Ref.[12], here we use the LWS representation, so that the spin-singlet two-spinon $s1$ fermions of momenta (i) $\vec{q}$ and (ii) $-\vec{q}$ involve (i) a spin-down spinon of momentum $\vec{q}$ and a spin-up spinon of momentum $-\vec{q}$ and (ii) a spin-down spinon of momentum $-\vec{q}$ and a spin-up spinon of momentum $\vec{q}$, respectively.

Within the LWS representation, a one-electron removal excitation breaks the spin-singlet spinon pair of a $s1$ fermion before the annihilation of a spin-down electron. The spin-down spinon of momentum $\vec{q}$ is then removed within the electron. The uncompensated spin-up spinon momentum $-\vec{q}$ is associated with that of a hole emerging in the $s1$ band at momentum $\vec{q}$. Indeed, the latter spinon decays into that momentum $-\vec{q}$ $s1$ band hole and a vanishing-momentum spin-up independent spinon. Hence one-electron excitations break spinon bond pairs whose spinons had momenta $\vec{q}$ and $-\vec{q}$ corresponding to their relative motion in the pair.

In turn, spinon pair breaking under spin excitations or excitations involving removal of two electrons with the same spin projection may introduce an extra momentum contribution that corresponds to the motion of the center of mass of the broken spin-singlet spinon pair. Under such excitations there emerge two holes in the $s1$ band at momenta $\vec{q}\,'$ and $\vec{q}\,''$ of the general form,

$$\vec{q}\,' = \vec{q} + \frac{1}{2}\delta\vec{q}; \quad \vec{q}\,'' = -\vec{q} + \frac{1}{2}\delta\vec{q}. \tag{26}$$

Here,

$$\vec{q} = \frac{1}{2}[\vec{q}\,' - \vec{q}\,'']\,; \quad \delta\vec{q} = \vec{q}\,' + \vec{q}\,''\,. \tag{27}$$

where $\vec{q}$ corresponds to the spinon relative motion in the pair and $\delta\vec{q}$ refers to the motion of the center of mass of the spinon pair.

That for the square-lattice quantum liquid both the c and $s1$ fermion discrete momentum values are good quantum numbers confirms the suitability of the present description in terms of occupancy configurations of the c and $s1$ effective lattices. Indeed, the c and $s1$ band discrete momentum values are the conjugate of the real-space coordinates of the c and $s1$ effective lattice, respectively. Are the approximations used in the construction of the $s1$ effective lattice inconsistent with the $s1$ band discrete momentum values being good quantum numbers? The answer is no. Indeed, such approximations concern the relative positions of the $j = 1, ..., N^2_{a_{s1}}$ sites of the $s1$ effective lattice[12,19,31]. They are only directly related to the shape of the $s1$ band boundary. They do not affect the $s1$ band discrete momentum values being good quantum numbers. At $x = 0$ the spin effective lattice is identical to the original square lattice and the $s1$ effective lattice is one of its two sub-lattices. Consistently, at $x = 0$ and $m = 0$ the boundary of the $s1$ momentum band is accurately known. Indeed, then the $s1$ band coincides with an antiferromagnetic reduced Brillouin zone of momentum area $2\pi^2$ such that $|q_{x_1}| + |q_{x_2}| \leq \pi$[19]. In turn, it is known that for $x > 0$ and $m = 0$ the the $s1$ band boundary encloses a smaller momentum area $(1-x)2\pi^2$ yet its precise shape remains an open issue. The related problems of the c and $s1$ momentum bands and corresponding energy dispersions and velocities are studied in Ref.[19].

For a number of sites $N^2_a \gg 1$ very large but finite that the description used in the studies of this paper refers to a $m = 0$ ground state is both for $x = 0$ and $x > 0$ a spin-singlet state[12]. For $m = 0$ and $x = 0$ this agrees with a theorem introduced and proved in Ref.[5]. The corresponding one- and two-electron subspace considered in this paper may be divided into a well-defined set of smaller subspaces spanned by neutral states. Such states conserve the eigenvalue $S_c = [1/2](1-x)N^2_a$ of the generator of the hidden $U(1)$ symmetry and the spin $S_s = 0, \frac{1}{2}, 1$ and thus conserve as well the number of sites of the $s1$ effective lattice $N^2_{a_{s1}} = [S_c + S_s]$. The set of energy eigenstates that span such subspaces are particular cases of the general momentum eigenstates $|\Phi_{U/4t}\rangle$ studied in Ref.[12]. The use of the general expression of such states leads to the following corresponding general form for the energy eigenstates $|\Psi_{U/4t}\rangle = |\Phi_{U/4t}\rangle$ that span the one- and two-electron subspace considered here,

$$|\Psi_{U/4t}\rangle = \frac{(\hat{S}^\dagger_s)^{L_{s,\,-1/2}}}{\sqrt{\mathcal{C}_s}}|\Phi_{LWS;U/4t}\rangle\,; \quad \mathcal{C}_s = \delta_{L_{s,\,-1/2},\,0} + \prod_{l=1}^{L_{s,\,-1/2}} l\,[\,L_s + 1 - l\,] = 1, 2, 4\,. \tag{28}$$

The LWS appearing in this equation reads,

$$|\Psi_{LWS;U/4t}\rangle = [|0_\eta; N^2_{a_\eta}\rangle][\prod_{\vec{q}\,'} f^\dagger_{\vec{q}\,',s1}|0_{s1}; N_{a^2_s}\rangle][\prod_{\vec{q}} f^\dagger_{\vec{q},c}|GS_c; 0\rangle]\,; \quad f^\dagger_{\vec{q}\,',s1} = \hat{V}^\dagger\,\mathcal{F}^\dagger_{\vec{q}\,',s1}\,\hat{V}\,; \quad f^\dagger_{\vec{q},c} = \hat{V}^\dagger\,\mathcal{F}^\dagger_{\vec{q},c}\,\hat{V}\,. \tag{29}$$

Here $\mathcal{F}^{\dagger}_{\vec{q}',s1}$ and $\mathcal{F}^{\dagger}_{\vec{q},c}$ are the creation operators of a $U/4t \rightarrow \infty$ $s1$ fermion of momentum $\vec{q}'$ and c fermion of momentum $\vec{q}$, respectively[12]. Moreover, $|0_\eta; N^2_{a_\eta}\rangle$ is the η-spin $SU(2)$ vacuum associated with $N^2_{a_\eta}$ independent $+1/2$ η-spinons, $|0_s; N^2_{a_s}\rangle$ is the spin $SU(2)$ vacuum associated with $N^2_{a_s}$ independent $+1/2$ spinons, and $|GS_c; 0\rangle$ is the c $U(1)$ vacuum. Such three vacua are invariant under the electron - rotated-electron unitary transformation, refer to the model global $[SU(2) \times SU(2) \times U(1)]/Z^2_2 = SO(3) \times SO(3) \times U(1)$ symmetry[4], and appear in the theory vacuum of Eq. (A3) of Appendix A. (In that equation, $|GS_c; 2S_c\rangle = \prod_{\vec{q}} f^{\dagger}_{\vec{q},c}|GS_c; 0\rangle$.)

The more general states $|\Phi_{U/4t}\rangle$ considered in Ref.[12] involve occupancy configurations of the remaining $\eta\nu$ fermion and $\nu > 1$ $s\nu$ fermion branches and $-1/2$ η-spinon occupancies absent in the expressions given in Eqs. (28) and (29). Importantly, the results of that reference concerning the subspaces A and B defined in it confirm that the states of form (28) and (29) are indeed energy eigenstates. Since they span all subspaces of the one- and two-electron subspace that conserve S_c and S_s, they span the latter subspace as well. In contrast, the momentum eigenstates generated by simple occupancy configurations of c and $\alpha\nu$ fermions and independent η-spinons and spinons of the larger set of states $\{|\Phi_{U/4t}\rangle\}$ considered in Ref.[12] are not in general energy eigenstates. As justified in that reference, the energy eigenstates are superpositions $|\Psi_{U/4t}\rangle = \sum_l C_l\,|\Phi_{U/4t;l}\rangle$ of a set of such states $\{|\Phi_{U/4t;l}\rangle\}$ with the same momentum eigenvalue. We recall that states with a single $s2$ fermion have also the general form provided Eqs. (28) and (29). As discussed above, the presence of that vanishing-energy, vanishing-momentum, and spin-neutral four-spinon object is accounted for the values of the numbers $[N^h_{s1} - 2S_s] = [S_c - S_s - N_{s1}] = 2N_{s2} = 0, 2$ of Eq. (19).

The energy eigenstates $|\Psi_{U/4t}\rangle$ of general form (28) that span the one- and two-electron subspace have numbers $N_{s2} = N^2_{a_{s2}} = 0, 1$ and $N_{s1} \approx N^2_{a_{s1}}$ such that $N^h_{s1} = [N^2_{a_{s1}} - N_{s1}] = 0, 1, 2$. Hence according to the results of Ref.[12] the lattice spacing $a_{s1} \approx \sqrt{2}\,a_s = \sqrt{2/(1-x)}\,a$ of Eq. (21) is directly related to the fictitious magnetic-field length l_{s1} associated with the field of Eq. (A2) of Appendix A. Indeed, in that subspace one has that $\langle n_{\vec{r}_j,s1}\rangle \approx 1$ and such a fictitious magnetic field reads $\vec{B}_{s1}(\vec{r}_j) \approx \Phi_0 \sum_{j' \neq j} \delta(\vec{r}_{j'} - \vec{r}_j)\,\vec{e}_{x_3}$. It acting on one $s1$ fermion differs from zero only at the positions of other $s1$ fermions. In the mean field approximation one replaces it by the average field created by all $s1$ fermions at position $\vec{r}_j$. This gives, $\vec{B}_{s1}(\vec{r}_j) \approx \Phi_0\, n_{s1}(\vec{r}_j)\,\vec{e}_{x_3} \approx \Phi_0\,[N^2_{a_{s1}}/L^2]\,\vec{e}_{x_3} = [\Phi_0/a^2_{s1}]\,\vec{e}_{x_3}$. One then finds that the number $N^2_{a_{s1}}$ of the $s1$ band discrete momentum values equals $[B_{s1}\,L^2]/\Phi_0$. In addition, the $s1$ effective lattice spacing a_{s1} is expressed in terms to the fictitious magnetic-field length $l_{s1} \approx a/\sqrt{\pi(1-x)}$ as $a^2_{s1} = 2\pi\,l^2_{s1}$. This is consistent with each $s1$ fermion having a flux tube of one flux quantum on average attached to it.

As further discussed in Ref.[19], for the present one- and two-electron subspace the $s1$ fermion problem is then related to the Chern-Simons theory[33]. Indeed the number of flux quanta being one is consistent with the $s1$ fermion and $s1$ bond-particle wave functions obeying Fermi and Bose statistics, respectively. Hence the composite $s1$ fermion consists of two spinons in a spin-singlet configuration plus an infinitely thin flux tube attached to it. Thus, each $s1$ fermion appears to carry a fictitious magnetic solenoid with it as it moves around in the $s1$ effective lattice.

III. LONG-RANGE ANTIFERROMAGNETIC ORDER AND SHORT-RANGE SPIRAL-INCOMMENSURATE SPIN ORDER FOR $x = 0$ AND $0 < x \ll 1$, RESPECTIVELY

Here we profit from the rotated-electron description used in the studies of this paper to address issues related to the occurrence for $m = 0$, zero temperature $T = 0$, and $N^2_a \rightarrow \infty$ of a long-range antiferromagnetic order and a short-range spiral-incommensurate spin order at $x = 0$ and for $0 < x \ll 1$, respectively. The emergence as $N^2_a \rightarrow \infty$ of a long-range antiferromagnetic order in the $x = 0$ and $m = 0$ ground state is associated with a spontaneous symmetry breaking. We argue that a condition for emergence of such a long-range antiferromagnetic order is that the spin effective lattice is identical to the original lattice. Such a condition is not met for small hole concentrations $0 < x \ll 1$.

A. Extension of the Mermin and Wagner Theorem to the half-filled Hubbard model for $U/4t > 0$

It is well known that for $U/4t \gg 1$ the spin degrees of freedom of the half-filled Hubbard model on a square lattice may be described by an isotropic spin-1/2 Heinsenberg model on a square lattice. It follows that the Mermin and Wagner Theorem[35] is valid for the former model at half filling and $U/4t \gg 1$. The theorem states that then there is no long-range antiferromagnetic order for finite temperatures $T > 0$ and $N^2_a \rightarrow \infty$.

Let us provide evidence that the Mermin and Wagner Theorem applies to the half-filled Hubbard model on a square lattice for all values $U/4t > 0$. The possibility of such an extension to $U/4t > 0$ is strongly suggested by evidence involving the transformation laws of the spin configurations under the electron - rotated-electron unitary transformation. We recall that in terms of the rotated electrons as defined in Section I and Ref.[12], the occupancy

configurations that generate the energy eigenstates $|\Psi_{U/4t}\rangle = \hat{V}^{\dagger}|\Psi_{\infty}\rangle$ are the same for all finite values $U/4t > 0$. Moreover, such rotated-electron occupancy configurations equal those that generate the corresponding energy eigenstates $|\Psi_{\infty}\rangle$ in terms of electrons in the $U/4t \rightarrow \infty$ limit.

The rotated-electron configurations that generate the energy eigenstates $|\Psi_{U/4t}\rangle$ that span the one- and two-electron subspace defined in this paper are much more complex than those associated with the simple form (28) and (29) in terms of c and $s1$ fermion operators. Indeed, the expression of their generators is in terms of rotated-electron creation operators is an involved problem. This follows from the expression of the spin-neutral two-spinon $s1$ fermion operators not being simple in terms of the rotated-electron operators[19,31]. This reveals that the electronic occupancy configurations that in the $U/4t \rightarrow \infty$ limit generate such energy eigenstates correspond to an involved problem as well. For $U/4t \rightarrow \infty$ the c fermion holes, spinons, and η-spinons are the "quasicharges", spins, and pseudospins, respectively, of Ref.[36]. For the Hubbard model on the square lattice in the one- and two-electron subspace the energy bandwidth of the $s1$ fermion dispersion vanishes for $U/4t \rightarrow \infty$ and the c fermion dispersion has in that limit the simple form $\epsilon_c(\vec{q}) = -2t\sum_{i=1}^{2}[\cos(q_{x_i}) - \cos(q_{Fcx_i})]$ in terms of the c band momentum components[19]. Here q_{Fcx_i} where $i = 1, 2$ are the components of the c Fermi momentum $\vec{q}_{Fc}$ defined in Ref.[19].

The use below of the following two properties provides strong evidence that the Mermin and Wagner Theorem holds for the half-filled Hubbard model on the square lattice for $U/4t > 0$: I) The $x = 0$ and $m = 0$ absolute ground state is in the limit $N_a^2 \rightarrow \infty$ invariant under the electron - rotated-electron unitary transformation[12,19]. Hence the occurrence for $N_a^2 \rightarrow \infty$ of long-range antiferromagnetic order as $U/4t \rightarrow \infty$, associated with that of the isotropic spin-1/2 Heisenberg model, implies the occurrence for $N_a^2 \rightarrow \infty$ of that long-range order for $U/4t > 0$ as well; II) Since in terms of rotated electrons single and double occupancy are good quantum numbers for $U/4t > 0$, the rotated-electron occupancy configurations that generate the energy eigenstates are more ordered than the corresponding electron occupancy configurations. It follows that the lack of long-range antiferromagnetic order in terms of the spins of the rotated electrons implies as well a lack of such an order in terms of the spins of the electrons whose occupancy configurations generate the same states.

The rotated-electron operator description of Ref.[12] has been constructed to inherently the electron occupancy configurations that for $U/4t \rightarrow \infty$ generate an energy eigenstate $|\Psi_{\infty}\rangle$ being identical to the rotated-electron occupancy configurations that for $U/4t > 0$ generate the energy eigenstates $|\Psi_{U/4t}\rangle = \hat{V}^{\dagger}|\Psi_{\infty}\rangle$ belonging to the corresponding V tower. Hence concerning the original-lattice rotated-electron occupancies, the Mermin and Wagner Theorem applies to all finite values of $U/4t > 0$: That for the occupancy configurations of the rotated-electron spins there is no long-range antiferromagnetic order for temperatures $T > 0$ and $N_a^2 \rightarrow \infty$ is an exact result. The above property II then implies that the lack of long-range antiferromagnetic order of the rotated-electron spins for $U/4t > 0$ and $T > 0$ implies a similar lack of such an order for the spins of the original electrons. Indeed, for finite values of $U/4t$ the spin occupancy configurations are more ordered for the rotated electrons than for the electrons.

This is also consistent with the emergence of a long-range antiferromagnetic order in the Hubbard model on a square lattice in the thermodynamic limit $N_a^2 \rightarrow \infty$ at hole concentration $x = 0$, temperature $T = 0$, and $U/4t > 0$. Indeed, there is a large consensus that in the thermodynamic limit $N_a^2 \rightarrow \infty$ long-range antiferromagnetic order occurs in the ground state of the related isotropic spin-1/2 Heisenberg model on the square lattice[23–25]. This implies that in the thermodynamic limit $N_a^2 \rightarrow \infty$ a similar long-range order sets in in the ground state of the half-filled Hubbard model on the square lattice at large $U/4t \gg 1$ values. Moreover, for $U/4t > 0$ a similar ground-state order occurs in that limit in the ground state of the latter model, in terms of the spins of the rotated electrons. That according to the above property I the $x = 0$ and $m = 0$ absolute ground state is in the limit $N_a^2 \rightarrow \infty$ invariant under the electron - rotated-electron unitary transformation then implies that in the thermodynamic limit $N_a^2 \rightarrow \infty$ and for $U/4t > 0$ a long-range antiferromagnetic order sets in in the ground state of the half-filled Hubbard model on the square lattice in terms of the spins of the electrons as well. This agrees with many previous studies of that model, as for instance those of Refs.[11,26–30]. As discussed below, there is strong evidence that both for $x = 0$, $T > 0$, and $U/4t > 0$ and for $0 < x \ll 1$, $T \geq 0$, and $U/4t > 0$ such a ground-state long-range order is replaced by a ground-state short-range spiral-incommensurate spin order.

B. $x = 0$ and $m = 0$ ground-state symmetry for $N_a^2 \rightarrow \infty$ and a necessary condition for its spontaneous symmetry breaking

Our above arguments provide strong evidence that provided that in the thermodynamic limit $N_a^2 \rightarrow \infty$ a long-range antiferromagnetic order occurs in the ground state of the related isotropic spin-1/2 Heisenberg model on the square lattice, a similar long range order sets in in that limit in the ground state of the half-filled Hubbard model on the square lattice for $U/4t > 0$. However, our goal is not providing a mathematical proof that in the thermodynamic limit $N_a^2 \rightarrow \infty$ long-range antiferromagnetic order occurs in the half-filled Hubbard model on the square lattice. Although there is no such a proof, there is a large consensus that it should be so[11,26–30]. An appropriate measure of such a

long-range order is the square of the staggered magnetization,

$$\langle\Psi_{GS}|\vec{\hat{M}}_s^{\,2}|\Psi_{GS}\rangle = \langle\Psi_{GS}|\left(\frac{1}{N_a^2}\sum_{j=0}^{N_a^2-1}\varepsilon_j\vec{\hat{s}}_{\vec{r}_j}\right)^2|\Psi_{GS}\rangle = \frac{1}{N_a^2}\sum_{j=0}^{N_a^2-1}\varepsilon_0\,\varepsilon_j\,C_j\,. \tag{30}$$

Here the spin operator $\vec{\hat{s}}_{\vec{r}_j}$ refers to the spin of an electron at the site of real-space coordinate $\vec{r}_j$ in the original lattice, C_j is the spin correlation function in the spin-singlet $S_s = 0$ and $x = 0$ ground state $|\Psi_{GS}\rangle$ of the model for $N_a^2 \gg 1$ very large but finite,

$$C_j = \langle\Psi_{GS}|\vec{\hat{s}}_{\vec{r}_0}\cdot\vec{\hat{s}}_{\vec{r}_j}|\Psi_{GS}\rangle\,, \tag{31}$$

and $\varepsilon_j = +1$ if j refers to the sub-lattice A. Otherwise $\varepsilon_j = -1$. This just compensates the sign of the antiferromagnetic correlation function (31). For $N_a^2 \gg 1$ finite and even the $x = 0$ and $m = 0$ ground state $|\Psi_{GS}\rangle$ appearing in Eqs. (30) and (31) has zero momentum.

The spin operator $\vec{\hat{s}}_{\vec{r}_j}$ appearing in Eqs. (30) and (31) has operator Cartesian components $\hat{s}^{x_1}_{\vec{r}_j}$, $\hat{s}^{x_2}_{\vec{r}_j}$, and $\hat{s}^{x_3}_{\vec{r}_j}$ and refers to the spin of an electron at the site of real-space coordinate $\vec{r}_j$. In turn, we denote the corresponding rotated spin or spinon operator by $\vec{s}_{\vec{r}_j}$ and its operator Cartesian components by $s^{x_1}_{\vec{r}_j}$, $s^{x_2}_{\vec{r}_j}$, and $s^{x_3}_{\vec{r}_j}$. It refers to the spin of a rotated electron at the site of real-space coordinate $\vec{r}_j$ whose components appear in Eqs. (7) and (9). Our spinons are such rotated spins.

Under the emergence of long-range antiferromagnetic order in the limit $N_a^2 \to \infty$, the square of the staggered magnetization $\langle\Psi_{GS}|\vec{\hat{M}}_s^{\,2}|\Psi_{GS}\rangle$ extrapolates to a finite asymptotic absolute value $|C_\infty|$ of the correlation function (31),

$$\lim_{N_a^2\to\infty}\langle\Psi_{GS}|\vec{\hat{M}}_s^{\,2}|\Psi_{GS}\rangle = |C_\infty|\,. \tag{32}$$

The related magnetic structure factor $S(\vec{k})$ is the Fourier transform of that correlation function,

$$S(\vec{k}) = \sum_{j=0}^{N_a^2-1} e^{i\vec{k}\cdot\vec{r}_j}C_j\,. \tag{33}$$

It can be measured directly in neutron scattering experiments[3,19]. As a result of its form (33), $S(\vec{\pi}) = N_a^2\langle\vec{\hat{M}}_s^{\,2}\rangle$ will grow linearly with the number of sites N_a^2 if there is long-range antiferromagnetic order for $N_a^2 \to \infty$,

$$\frac{S(\vec{\pi})}{N_a^2} = \langle\Psi_{GS}|\vec{\hat{M}}_s^{\,2}|\Psi_{GS}\rangle = \frac{m_{AF}^2}{3} + \mathcal{O}(1/N_a)\,. \tag{34}$$

Here the sub-lattice magnetization $m_{AF} = \lim_{N_a^2\to\infty} 3\langle\vec{\hat{M}}_s^{\,2}\rangle = 3|C_\infty|$ plays the role of antiferromagnetic order parameter.

The large scale DQMC calculations of Ref.[11] provide useful information on the effective bandwidth, momentum distribution, and magnetic correlations of the half-filled Hubbard model on the square lattice. They employ the DQMC method, which provides an approximation-free solution of the such a model on square lattices large enough to use finite-size scaling to, for example, reliably extract the sub-lattice magnetization $m_{AF} = 3|C_\infty|$ as a function of $U/4t$. Such Monte Carlo calculations as well the random-phase approximation results of Ref.[27] reveal that m_{AF} vanishes for $U/4t \to 0$ and is an increasing function of $U/4t$ that for approximately $U/4t \approx 2$ saturates to the value $m_{AF}^{HM} \approx 0.614$ of the isotropic spin-1/2 Heisenberg model on the square lattice determined in Ref.[25]. The quantum Monte Carlo DQMC results of Ref.[11] are an improvement of the corresponding results of Monte Carlo simulations of Ref.[26], which predicted a lower value for the saturated m_{AF}. Below we relate the sub-lattice magnetization m_{AF} to an energy scale that can as well be used as antiferromagnetic order parameter. Combining that relation with the behavior $m_{AF} = m_{AF}^{HM} \approx 0.614$ for $U/4t \gg 1$, we find the following approximate limiting behaviors,

$$\begin{aligned} m_{AF} &\approx \frac{8^2t}{U}\,e^{-\pi\sqrt{\frac{4t}{U}}}\,, \quad U/4t \ll 1\,, \\ &\approx m_{AF}^{HM} - \frac{1}{4}\left(\frac{2-U/4t}{2\ln 2}\right)^2\,, \quad u_0 \leq U/4t \leq 2\,, \\ &\approx m_{AF}^{HM}\,, \quad U/4t > 2\,. \end{aligned} \tag{35}$$

where

$$m_{AF}^{HM} \approx \frac{2e^1}{\pi^2} + \frac{1}{4}\left(\frac{2-u_0}{2\ln 2}\right)^2 \approx 0.6142\,. \tag{36}$$

The expression given in Eq. (35) for $u_0 \leq U/4t \leq 2$ is also valid for $0 \leq (u_0 - U/4t) \ll 1$ where u_0 is a $U/4t$ value found below to read $u_0 \approx 1.302$. Alike in Ref.[11], Eqs. (35) and (36) refer to units where the classical Néel state has $m_{AF} = 1$. In Ref.[25] units are used where that state has $m_{AF} = 1/2$. In the latter units the parameter (36) reads instead ≈ 0.3071, consistently with the results of that reference.

When expressed in terms of rotated-electron creation and annihilation operators, the Hamiltonian of the Hubbard model on the square lattice (1) has an infinite number of terms, as given in Eq. (5). For the half-filled model in the one- and two-electron subspace with both no rotated-electron double occupancy and no rotated-hole double occupancy the c fermion band is full for the ground state. Moreover, the excitations involving the emergence of c fermion holes are gapped. In the one- and two-electron subspace the model Hamiltonian (5) may then be expressed only in terms of spinon operators $\vec{s}_{\vec{r}_j}$ whose operator components $s^l_{\vec{r}_j}$ are given in Eq. (7). Consistently with the related results of Ref.[7], one finds that up to fifth order in t/U the Hamiltonian (5) has in terms of such spin operators the following form,

$$\begin{aligned}
H \;=\; & \frac{t^2}{2U}\sum_{\langle j_1 j_2\rangle}(\vec{s}_{\vec{r}_{j_1}}\cdot\vec{s}_{\vec{r}_{j_2}} - 1) - \frac{2t^4}{U^3}\sum_{\langle j_1 j_2\rangle}(\vec{s}_{\vec{r}_{j_1}}\cdot\vec{s}_{\vec{r}_{j_2}} - 1) \\
& + \frac{t^4}{2U^3}\sum_{j_1,j_2,j_3} D_{j_1,j_2}D_{j_2,j_3}(\vec{s}_{\vec{r}_{j_1}}\cdot\vec{s}_{\vec{r}_{j_3}} - 1) \\
& + \frac{t^4}{8U^3}\sum_{j_1,j_2,j_3,j_4} D_{j_1,j_2}D_{j_2,j_3}D_{j_3,j_4}D_{j_4,j_1}(1 - \vec{s}_{\vec{r}_{j_1}}\cdot\vec{s}_{\vec{r}_{j_2}} \\
& - \vec{s}_{\vec{r}_{j_1}}\cdot\vec{s}_{\vec{r}_{j_3}} - \vec{s}_{\vec{r}_{j_1}}\cdot\vec{s}_{\vec{r}_{j_4}} - \vec{s}_{\vec{r}_{j_2}}\cdot\vec{s}_{\vec{r}_{j_3}} - \vec{s}_{\vec{r}_{j_2}}\cdot\vec{s}_{\vec{r}_{j_4}} - \vec{s}_{\vec{r}_{j_3}}\cdot\vec{s}_{\vec{r}_{j_4}}) \\
& + \frac{5t^4}{8U^3}\sum_{j_1,j_2,j_3,j_4} D_{j_1,j_2}D_{j_2,j_3}D_{j_3,j_4}D_{j_4,j_1}[(\vec{s}_{\vec{r}_{j_1}}\cdot\vec{s}_{\vec{r}_{j_2}})(\vec{s}_{\vec{r}_{j_3}}\cdot\vec{s}_{\vec{r}_{j_4}}) \\
& + (\vec{s}_{\vec{r}_{j_1}}\cdot\vec{s}_{\vec{r}_{j_4}})(\vec{s}_{\vec{r}_{j_2}}\cdot\vec{s}_{\vec{r}_{j_3}}) - (\vec{s}_{\vec{r}_{j_1}}\cdot\vec{s}_{\vec{r}_{j_3}})(\vec{s}_{\vec{r}_{j_2}}\cdot\vec{s}_{\vec{r}_{j_4}})]\,.
\end{aligned} \tag{37}$$

Here $\langle j_1 j_2\rangle$ refers to a summation running over nearest-neighboring sites and $D_{j,j'} = 1$ for the real-space coordinates $\vec{r}_j$ and $\vec{r}_{j'}$ corresponding to nearest-neigboring sites and $D_{j,j'} = 0$ otherwise. Analysis of the interactions in spin space of the Hamiltonian (37) reveals that some of its terms do not introduce frustration whereas other do. However, at half filling the spin interactions of the Hamiltonian (37) including those of all higher order contributions do not destroy the sub-lattice magnetization m_{AF}. They merely destabilize the classical Néel state, lessening the sub-lattice magnetization from its classical magnitude $m_{AF} = 1$.

That as obtained by different authors and methods[11,23,26,27] the sub-lattice magnetization m_{AF} of Eqs. (34) and (35) is indeed finite for the Hubbard model on the square lattice at $U/4t > 0$ provides strong evidence that for $N_a^2 \rightarrow \infty$ the spin correlation function (31) has long-range antiferromagnetic order. In contrast to 1D, the quantum fluctuations associated with the interactions in spin space of the Hamiltonian (37) and its higher-order terms are not strong enough to destroy it. In turn, the exact Mermin-Wagner Theorem[35] implies that at finite temperatures thermal fluctuations destroy such an order of the square-lattice model.

A stronger confirmation is obtained by the scaling of the spectrum itself. It is an illustration of the mechanism of spontaneous symmetry breaking. Anderson was the first to point out that the spontaneous symmetry breaking mechanism that occurs in the thermodynamic limit $N_a^2 \rightarrow \infty$ involves a whole tower of low-lying energy eigenstates of the finite system[37]. They collapse in that limit onto the ground state. One may investigate which energy eigenstates couple to the exact finite $N_a^2 \gg 1$ and $x = 0$ and $m = 0$ ground state $|\Psi_{GS}\rangle$ via the operator of the staggered magnetization $\hat{M}^l_s$. Here $l = \pm, x_3$. We insert a complete set of energy eigenstates as follows,

$$\langle\Psi_{GS}|(\hat{M}^l_s)^2|\Psi_{GS}\rangle = \sum_i \langle\Psi_{GS}|\hat{M}^l_s|\Psi_i\rangle\langle\Psi_i|\hat{M}^l_s|\Psi_{GS}\rangle = \sum_i |\langle\Psi_{GS}|\hat{M}^l_s|\Psi_i\rangle|^2\,;\quad l = \pm, x_3\,. \tag{38}$$

Only excited energy eigenstates $|\Psi_i\rangle$ with momentum $\vec{k} = \vec{\pi}$ and quantum numbers $S_\eta = 0$, $S_c = N_a^2/2$, $S_s = 1$, and $S^{x_3}_s = 0, \pm 1$ corresponding to $l = x_3, \pm$ contribute to the sum of Eq. (38). We emphasize that the quantum numbers $S_\eta = 0$ and $S_c = N_a^2/2$ remain unchanged and thus are the same as for the ground state $|\Psi_{GS}\rangle$. We denote by $|\Psi_{1T}\rangle$ the lowest $S_s = 1$, $S_\eta = 0$, $S_c = N_a^2/2$, and $\vec{k} = [\pi, \pi]$ spin-triplet state whose excitation energy behaves

as $1/N_a^2$ for finite $N_a^2 \gg 1$. For the range $U/4t > u_0 \approx 1.3$ of interest for the studies of Ref.[19] the contribution from such a lowest spin triplet state is by far the largest: For instance for approximately $U/4t > 2$ the matrix-element square $|\langle \Psi_{GS}|\hat{M}_s^l|\Psi_{1T}\rangle|^2$ exhausts the sum in Eq. (38) by more than 98.7%. (This is the value found by exact diagonalization for the related spin-1/2 Heisenberg model on the square lattice in Ref.[24]. As similar result is expected for approximately $U/4t > u_0 \approx 1.3$.)

The special properties with respect to the lattice symmetry group of the lowest energy eigenstates contributing to the linear Goldstone modes of the corresponding $S_s = 1$ spin-wave spectrum reveal the space-symmetry breaking of the $N_a^2 \rightarrow \infty$ ground state. In the present case of the half-filled Hubbard model on the square lattice the translation symmetry is broken. Hence both the $\vec{k} = [0,0]$ and $\vec{k} = [\pi,\pi]$ momenta appear among the lowest energy eigenstates contributing to the linear Goldstone modes of the $S_s = 1$ spin-wave spectrum.

The c and $s1$ fermion description can be used to derive such a spin-wave spectrum. For $x = 0$ and $m = 0$ it is generated in Ref.[19] in terms of simple two-$s1$-fermion-hole processes. The investigations of that reference confirm that at $x = 0$ the spin-wave spectrum includes linear Goldstone modes at momenta $\vec{k} = [0,0]$ and $\vec{k} = [\pi,\pi]$. That the transverse spin-spin correlation function contains gapless poles, as predicted by the Goldstone Theorem, is consistent with in the limit $N_a^2 \rightarrow \infty$ the ground state breaking the continuous spin $SU(2)$ rotational invariance of the Hamiltonian. The corresponding spin-wave spectrum is plotted in Fig. 1 of Ref.[19] for the half-filled Hubbard model on the square lattice in the thermodynamic limit $N_a^2 \rightarrow \infty$. (As mentioned above, for large N_a^2 the lowest $\vec{k} = [\pi,\pi]$ excitation energy vanishes as $1/N_a^2$.) The occurrence of linear Goldstone modes at momenta $\vec{k} = [0,0]$ and $\vec{k} = [\pi,\pi]$ in the theoretical spin-wave spectrum derived in Ref.[19] explicitly confirms that the results of the c and $s1$ fermion description used in the studies of this paper are fully consistent with for $x = 0$, $m = 0$, and temperature $T = 0$ long-range antiferromagnetic setting in as $N_a^2 \rightarrow \infty$.

Importantly, for $U/4t \approx 1.525$ and $t \approx 295$ meV the spin-wave spectrum of the parent compound La_2CuO_4 (LCO)[3] is quantitatively described by the corresponding theoretical spectrum derived in Ref.[19] in terms of simple spinon pair breaking $s1$ fermion processes. Within the present status of the scheme used in the studies of that reference one cannot calculate explicitly matrix elements of the two-electron spin-triplet operator between energy eigenstates and corresponding spectral-weight distributions. The $x = 0$ and $m = 0$ results of Ref.[19] on the spin-wave spectrum of the parent compound LCO profit from combination of the c and $s1$ fermion description with the complementary method of Ref.[38]. They reveal that the microscopic mechanisms that generate the coherent spectral-weight spin-wave energy spectrum are in terms of spinon pair breaking $s1$ fermion processes very simple. Indeed the two-spinon $s1$ fermion description renders a complex many-electron problem involving summation of an infinite set of ladder diagrams[38] into a non-interacting two-$s1$-fermion-hole spectrum, described by simple analytical expressions.

Within the semi-classical description of spin waves, they can be pictured as long wave-length twists of the order parameter. In turn, within the present quantum description a spinon bond pair of a spin-singlet two-spinon $s1$ fermion is broken, giving rise to two independent spin-up spinons or two independent spin-down spinons. All remaining spinons in the problem remain confined with spin-neutral two-spinon $s1$ fermions. The two deconfined spinons are invariant under the electron - rotated-electron unitary transformation. Thus their spin-triplet excite-state occupancies correspond to an isolated vanishing-energy and vanishing-momentum mode below a continuum of two-$s1$-fermion-hole excitations. Indeed, the momenta $\pm\vec{q}$ corresponding to the spinon relative motion in the spinon pair of the broken $s1$ fermion are transferred over to two holes, respectively, that emerge in the $s1$ band. Under spin-triplet excitations such a two-spinon $s1$ fermion breaking may introduce an extra momentum contribution $\delta\vec{q}$. It corresponds to the motion of the center of mass of the spinon broken pair. In the latter case the two emerging $s1$ band holes have momenta $\vec{q}\,'$ and $\vec{q}\,''$ given in Eqs. (26) and (27).

As found in Ref.[19], the processes associated with most momenta $\vec{q}\,'$ and $\vec{q}\,''$ lead to an incoherent background of spin spectral weight. In turn, the spin coherent spectral-weight distribution refers to the spin-wave spectrum. The processes that generate such a coherent spin weight are such that one of the $s1$ band momenta $\vec{q}\,'$ and $\vec{q}\,''$ belongs to the boundary line and the other points in a nodal direction. That some of the spin spectral weight is incoherent is consistent with the sub-lattice magnetization obeying the inequality $m_{AF} < 1$, rather than reading $m_{AF} = 1$, as for the classical Néel state. In turn, we argue below that the spin spectral weight is fully incoherent for spin excitations of $m = 0$ and $x > 0$ ground states.

In the thermodynamic limit $N_a^2 \rightarrow \infty$ a large number of low-lying energy eigenstates $|\Psi_i\rangle$ with momentum $\vec{k} = \vec{\pi}$ and quantum numbers $S_\eta = 0$, $S_c = N_a^2/2$, $S_s = 1$, and $S_s^{x_3} = 0, \pm 1$ that contribute to the sum of Eq. (38) converge to the corresponding $N_a^2 \gg 1$ finite ground state. To illustrate the mechanism of spontaneous symmetry breaking, we consider for simplicity that the lowest-energy spin triplet state $|\Psi_{1T}\rangle$ belonging to that set of energy eigenstates gives rise to such a symmetry breaking. Indeed, for intermediate and large $U/4t$ values such a state exhausts the sum in Eq. (38) by more than 98.7%. However, the lower broken symmetry of the final ground state is the same independently of the number of low-lying states considered in the analysis of the problem. In the presence of a small staggered field $\vec{B}_s$

in the x_3-direction, a new ground state emerges due to the additional term $M_s^{x_3} B_{x_3}$ in the Hamiltonian. This state,

$$|\Psi_{b-GS}\rangle \approx C_{GS}|\Psi_{GS}\rangle + C_{1T}|\Psi_{1T}\rangle\,, \tag{39}$$

has a finite staggered magnetization,

$$M_s = \langle\Psi_{b-GS}|\hat{M}_s^z|\Psi_{b-GS}\rangle = 2C_{GS}C_{1T}\langle\Psi_{GS}|\hat{M}_s^z|\Psi_{1T}\rangle\,. \tag{40}$$

In turn, $\langle\Psi_{GS}|\hat{M}_s^z|\Psi_{GS}\rangle = 0$ and $\langle\Psi_{1T}|\hat{M}_s^z|\Psi_{1T}\rangle = 0$. The new ground state $|\Psi_{b-GS}\rangle$ has not a well defined spin S_s, yet it has the same quantum numbers $S_\eta = 0$ and $S_c = N_a^2/2$ as the spin-singlet ground state $|\Psi_{GS}\rangle$.

In the thermodynamic limit $N_a^2 \rightarrow \infty$, the system assumes the largest possible magnetization for arbitrarily small staggering field $\vec{B}_s$, so that $C_{GS} = C_{1T} = 1/\sqrt{2}$ and thus $M_s = \langle\Psi_{GS}|\hat{M}_s^z|\Psi_{1T}\rangle$. The state $|\Psi_{b-GS}\rangle$ of Eq. (39) is contained in a reduced subspace spanned by $|\Psi_{GS}\rangle$ and $|\Psi_{1T}\rangle$. In such a reduced subspace the unity partition operator reads $\approx |\Psi_{GS}\rangle\langle\Psi_{GS}| + |\Psi_{1T}\rangle\langle\Psi_{1T}|$. We then obtain the following staggered magnetization squared,

$$M_s^2 = \langle\Psi_{b-GS}|\hat{M}_s^z|\Psi_{b-GS}\rangle^2 = \langle\Psi_{GS}|(\hat{M}_s^z)^2|\Psi_{GS}\rangle\,. \tag{41}$$

It follows that the staggered magnetization squared in the $N_a^2 \rightarrow \infty$ ground state $|\Psi_{b-GS}\rangle$ with broken symmetry is identical to the long-range antiferromagnetic order of the correlation function in the spin-singlet $N_a^2 \gg 1$ ground state $|\Psi_{GS}\rangle$, consistently with Eq. (32). Indeed, the studies of Ref.[12] reveal that for a number of sites $N_a^2 \gg 1$ large but finite the $m = 0$ ground states are spin-singlet states. For the present case of a $m = 0$ and $x = 0$ ground state this agrees with an exact theorem introduced and proved in Ref.[5].

The new ground state $|\Psi_{b-GS}\rangle$ of Eq. (39) is a superposition of states with different spin S_s and thus breaks the Hamiltonian spin $SU(2)$ symmetry contained in its global $SO(3) \times SO(3) \times U(1) = [SU(2) \times SU(2) \times U(1)]/Z_2^2$ symmetry. Specifically, the spin rotational symmetry $SU(2)$ is spontaneously broken to $U(1)$ by the formation of the staggered magnetization. In turn, the new ground state has the same quantum numbers $S_\eta = 0$ and $S_c = N_a^2/2$ as the spin-singlet ground state $|\Psi_{GS}\rangle$. Therefore, the corresponding η-spin symmetry $SU(2)$ and c fermion symmetry $U(1)$, respectively, are not broken. A similar result is obtained if besides $|\Psi_{GS}\rangle$ and $|\Psi_{1T}\rangle$, the new ground state $|\Psi_{b-GS}\rangle$ contains a larger set of low-lying energy eigenstates $|\Psi_i\rangle$ with momentum $\vec{k} = \vec{\pi}$ and quantum numbers $S_\eta = 0$, $S_c = N_a^2/2$, $S_s = 1$, and $S_s^{x_3} = 0, \pm 1$ other than $|\Psi_{1T}\rangle$. Hence rather than $SO(3) \times SO(3) \times U(1)$, the symmetry of new ground state $|\Psi_{b-GS}\rangle$ is $[U(2) \times U(1)]/Z_2^2 = [SO(3) \times U(1) \times U(1)]/Z_2 = [SU(2) \times U(1) \times U(1)]/Z_2^2$.

Consistently with the studies of the $x = 0$ two-spinon $s1$ fermion pairing energy of Ref.[19], in the Hubbard model on the square lattice state configurations such that $N_{a_\eta}^2 = [N_a^2 - 2S_c] = 0$ and thus $N_{a_s}^2 = N_a^2$ exist below an energy scale $\mu^0 \equiv \lim_{x\rightarrow 0}\mu$. Such an energy scale refers to the spin degrees of freedom yet it equals one half the charge Mott-Hubbard gap. The latter gap defines the range $\mu \in (-\mu^0, \mu^0)$ of the chemical potential μ at $x = 0$ and $m = 0$[12,19]. The energy scale μ^0 may be used as order parameter of the long-range antiferromagnetic order. It equals the excitation energy below which such an order exists in the limit $N_a^2 \rightarrow \infty$ at $m = 0$, $x = 0$, and zero temperature $T = 0$. The limiting behaviors of μ^0 are approximately the following,

$$\begin{aligned}
\mu^0 &\approx 32\,t\,e^{-\pi\sqrt{\frac{4t}{U}}}\,, \quad U/4t \ll 1\,, \\
&\approx \frac{2e^1\,t}{\pi}\sqrt{1 + (U/4t - u_0)}\,, \quad u_0 \leq U/4t \leq u_1\,, \\
&\approx [U/2 - 4t]\,; \quad U/4t \gg 1\,.
\end{aligned} \tag{42}$$

It vanishes $\mu^0 \rightarrow 0$ for $U/4t \rightarrow 0$ and is finite and an increasing function of $U/4t$ for $U/4t$ finite. For $U/4t \rightarrow \infty$ it behaves as $\mu^0 \approx U/2 \rightarrow \infty$. This is why in that limit, when the spin degrees of freedom of the half-filled Hubbard model are described by the isotropic spin-1/2 Heisenberg model, the state configurations for which $N_{a_s}^2 = N_a^2$ exist at any finite energy.

The behavior $\mu_0(U/4t) \approx \mu_0(u_0)\sqrt{1 + (U/4t - u_0)}$ reported in Eq. (42) is expected to be a good approximation for the intermediate $U/4t$ range $U/4t \in (u_0, u_1)$ of interest for the square-lattice quantum liquid studies of Ref[19]. Here $u_0 \approx 1.302$ and $u_1 \approx 1.600$. The approximate magnitude $\mu_0(u_0) \approx [2e^1/\pi]\,t$ is that consistent with the relation $\mu_0(u_0) \approx \mu_0(u_*)/\sqrt{1 + (u_* - u_0)}$. The value $U/4t = u_* = 1.525$ is that at which the studies of that reference lead by a completely different method to $\mu_0(u_*) \approx 566\,\mathrm{meV}$ for $t = 295\,\mathrm{meV}$ and $U/4t \approx u_* = 1.525$. The use of $\mu_0(u_0) \approx [2e^1/\pi]\,t$ in the formula $\mu_0(U/4t) \approx \mu_0(u_0)\sqrt{1 + (U/4t - u_0)}$ leads for $t = 295\,\mathrm{meV}$, $U/4t \approx u_* = 1.525$, and $u_0 = 1.302$ to nearly the same magnitude, $\mu_0(u_*) \approx 565\,\mathrm{meV}$. In turn, the value $U/4t = u_0 = 1.302$ is that at which the energy parameter $2\Delta_0$ is found below to reach its maximum magnitude. That energy parameter such that $2\Delta_0 < \mu_0$ for $U/4t > 0$ is the energy below which the short-range incommensurate-spiral spin order considered below survives for $0 < x \ll 1$, $m = 0$, and zero temperature $T = 0$.

We make the reasonable assumption that at $T = 0$ the energy parameter μ^0 and the sub-lattice magnetization m_{AF} of Eq. (35) scale in the same way as follows,

$$\mu^0 = U\, m_{AF}\, \alpha^0 \,. \tag{43}$$

A naive spin-density wave mean-field approach[27] leads to the relation $\mu^0 = [U/2]\, m_{AF}$. In turn, in the case of the relation (43) the coefficient $\alpha^0 \equiv \mu^0/[U\, m_{AF}]$ has the following limiting behaviors,

$$\begin{aligned} \alpha^0 &= 0.500\,, \quad U/4t \ll 1\,, \\ &\approx 0.603\,, \quad U/4t = u_0 \approx 1.302\,, \\ &\approx 0.536\,, \quad U/4t = u_* \approx 1.525\,, \\ &\approx 0.519\,, \quad U/4t = u_1 \approx 1.600\,, \\ &= \frac{1}{2m_{AF}^{HM}} \approx 0.814\,, \quad U/4t \gg 1\,. \end{aligned} \tag{44}$$

The physical quantities m_{AF} of Eq. (35), $U\, m_{AF}$, and μ^0 of Eq. (42) are increasing functions of $U/4t$. In turn, $\alpha^0 = \mu^0/U\, m_{AF}$ is a monotonous function of $U/4t$ with both minima and maxima. In the limit $U/4t \rightarrow 0$ the effects of all fluctuations vanish and the value $\alpha^0 = 1/2$ is that predicted by mean-field theory relation $\mu^0 = [U/2]\, m_{AF}$. As a function of $U/4t$, the coefficient α^0 first increases until reaching a maximum at a $U/4t$ value below u_0. Interestingly, in the intermediate range $U/4t \in (u_0, u_1)$ it is a decreasing function of $U/4t$. It reaches a minimum value larger than 0.500 and smaller than 0.519 at a $U/4t$ magnitude laying between $U/4t = u_1 \approx 1.6$ and $U/4t = 2$. It then becomes an increasing function of $U/4t$, reaching the value $\alpha^0 \approx 0.814$ for $U/4t \gg 1$. Since $\mu^0/U \rightarrow 1/2$ as $U/4t \rightarrow \infty$, note that the corresponding $U/4t \gg 1$ expression $\alpha^0 = 1/[2m_{AF}]$ would give $\alpha^0 = 1/2$ if the m_{AF} value was that of the classical Néel state $m_{AF} = 1$, rather than that of the spin-1/2 Heisenberg model $m_{AF} = m_{AF}^{HM} \approx 0.6142$.

Consistently with for the Hubbard model on a square lattice μ^0 being the energy below which the long-range antiferromagnetic order exists in the limit $N_a^2 \rightarrow \infty$ at $x = 0$, $m = 0$, and zero temperature $T = 0$, the limiting behaviors $\mu^0 \approx 32\, t\, e^{-2\pi\sqrt{t/U}}$ and $\mu^0 \approx U/2$ given in Eq. (42) for $U/4t \ll 1$ and $U/4t \gg 1$, respectively, are those of the zero-temperature spin gap of Eq. (13) of Ref.[29]. Within the operator description used in this paper the c fermions and spinon occupancies generate the state representations of the groups $U(1)$ and spin $SU(2)$, respectively, in the model global $SO(3) \times SO(3) \times U(1) = [SU(2) \times SU(2) \times U(1)]/Z_2^2$ symmetry. In turn, the studies of Ref.[30] isolate strongly fluctuating modes generated by the Hamiltonian (1) Hubbard term according to the charge $U(1)$ and spin $SU(2)$ symmetries. Within the gauge transformation of that reference, the strongly correlated problem is casted into a system of noninteracting "h fermions" submerged in the bath of strongly fluctuating $U(1)$ and $SU(2)$ gauge potentials. Those couple to fermions via hopping term plus the Zeeman-type contribution with a massive field $\varrho(\vec{r}_j\tau)$. Within the description of that reference a $U(1)$ and $SU(2)$ gauge transformation is used to factorize the charge and spin contribution to the original electron operator in terms of the emergent gauge fields. The $U(1)$ charge h fermions and $SU(2)$ spins of Ref.[30] refer to the c fermions and spinons, respectively, of our description. In what the relation of the energy scale of Eq. (42) to the results of that reference is concerned, in the $x = 0$ antiferromagnetic phase the above massive field $\varrho(\vec{r}_j\tau)$ assumes the staggered form,

$$\varrho(\vec{r}_j\tau) = \mu_0\, e^{i\vec{\pi}\cdot\vec{r}_j} \,. \tag{45}$$

The description of Ref.[30] is valid for large $U/4t$ values, so that $\mu_0 \approx U/2$, as given in Eq. (42). In turn, the c fermions and spinons of this paper are directly related to the rotated electrons of the description of Ref.[12], whose double occupancy is a good quantum number for $U/4t > 0$. This is why the energy scale μ_0 of Eq. (45) is here well defined for the whole range of $U/4t$ values. Consistently, $\mu^0 \approx 32\, t\, e^{-\pi\sqrt{\frac{4t}{U}}} \rightarrow 0$ and thus $\rho(\vec{r}_j\,\tau) \rightarrow 0$ for $U/4t \rightarrow 0$ upon the disappearance of the long-range antiferromagnetic order, as given in Eq. (42).

C. Short-range incommensurate-spiral spin order at $x = 0$ and $0 < T \ll T_0^*$ and for $0 < x \ll 1$ and $0 \leq T \ll T_0^*$

Here it is argued that the spin effective lattice being identical to the original lattice is a necessary condition for the emergence of a ground-state long-range antiferromagnetic order in the limit $N_a^2 \rightarrow \infty$. Moreover, it follows from the property II of Section III-A that since the ground-state rotated-electron occupancy configurations are for finite values of $U/4t$ more ordered than those of the electrons generating the same state, a lack of long-range antiferromagnetic order of the rotated-electron spins in the limit $N_a^2 \rightarrow \infty$ for $N_{a_s}^2/N_a^2 < 1$ would imply a similar lack of long-range antiferromagnetic order for the spins of the original electrons as $N_a^2 \rightarrow \infty$. The inequality $N_{a_s}^2/N_a^2 < 1$ applies to the $x > 0$ and $m = 0$ ground states. For those the spin effective lattice is different from the original lattice, in contrast to that of the absolute $x = 0$ and $m = 0$ ground state.

1. The general effects of hole doping accounting for the hidden global $U(1)$ symmetry

Quantum-Monte Carlo methods, when applicable, are the only unbiased tools for quantitative studies of the effects of a small hole concentration x in the physics of the Hubbard model on the square lattice. Unfortunately, some of the interactions that become active for $x > 0$ cannot be studied by Quantum-Monte Carlo simulations due to the well-known "sign problem". While part of our results are argued on phenomenological grounds, taking account for the effects of the hidden global $U(1)$ symmetry found recently for the Hubbard model on any bipartite lattice in Ref.[4] introduces a new scenario and framework, which may be useful for future quantitative studies of the square-lattice model. In addition, such a new scenario allows the preliminary qualitative discussion of the problem presented in this paper.

In accordance to a general theorem proved in Ref.[39], at half filling the terms of the Hamiltonian (5) expansion in t/U with odd powers in t vanish due to the particle-hole symmetry and the resulting invariance of the spectrum under $t \rightarrow -t$. For instance, the $x = 0$ and $m = 0$ Hamiltonian terms of Eq. (37) result only from the terms of order t^2 and t^4 of the Hamiltonian (6) of Ref.[13]. (The T_0 and $T_{\pm 1}$ operators of that reference include a factor t absent in the corresponding operators of Eq. (2).) In turn, for finite hole concentration $x > 0$ and vanishing spin density $m = 0$ the expansion in powers of t/U of the Hamiltonian (5) involves terms with odd powers in t, absent at $x = 0$. We argue that the emergence of such new terms absent at $x = 0$ along with related effects associated with changes in the spin effective lattice upon "turning on" the hole concentration x destroy the sub-lattice magnetization m_{AF}.

Expression of the Hamiltonian of the Hubbard model on the square lattice (1) in terms of rotated-electron creation and annihilation operators leads to the Hamiltonian (5), which has an infinite number of terms. Its expansion up to fifth order in t/U leads for the $x = 0$ half-filled Hubbard model in the one- and two-electron subspace to the Hamiltonian expression given in Eq. (37), which involves only spinon operators. In turn, for $x > 0$ the Hamiltonian (5) may be expressed in terms of c fermion operators, η-spinon operators, and spinon operators. This is done by the use of the expressions provided in Eq. (A1) of Appendix A for the rotated-electron operators in terms of such operators. The uniquely obtained Hamiltonian also has an infinite number of terms and thus is rather complex.

The problem slightly simplifies for the $x > 0$ Hamiltonian (5) in the one- and two-electron subspace. In terms of rotated-electron creation and annihilation operators, its terms generated up to fourth order in t/U are for $x > 0$ and within a unitary transformation the equivalent to the $t - J$ model with ring exchange and various correlated hoppings[13]. Moreover, in the one- and two-electron subspace such an Hamiltonian may be expressed in terms of only c fermion operators and spinon operators. The rotated quasi-spin operators are given by $q^l_{\vec{r}_j} = s^l_{\vec{r}_j} + p^l_{\vec{r}_j}$ where $l = \pm, z$. Here $s^l_{\vec{r}_j}$ and $p^l_{\vec{r}_j}$ are the spinon local operators and η-spinon local operators, respectively, given in Eq. (7). Since in the one- and two-electron subspace there are no rotated-electron doubly occupied sites, the η-spin effective lattice is empty and the operator $p^l_{\vec{r}_j}$ plays no active role. However, the obtained Hamiltonian expression is for $x > 0$ much more involved than that given in Eq. (37) for $x = 0$ and is omitted here. In addition to involving spinon operators, it contains c fermion operators and its number of terms is much larger than for $x = 0$. Moreover, it involves c fermion - spinon interactions and both non-frustated isotropic spinon interactions and spinon interactions with some degree of frustration. Hence such interactions cannot be studied by Quantum-Monte Carlo simulations due to the "sign problem".

In such an involved $x > 0$ Hamiltonian expression the c fermion operators act onto the c effective lattice occupancies and the spinon operators act onto the spin effective lattice occupancies. (The c fermion operators commute with the spinon operators.) Also in the $x > 0$ Hamiltonian (5) general expression containing an infinite number of terms, the c fermion operators act onto the c effective lattice occupancies, the η-spinon operators act onto the η-spin effective lattice occupancies, and the spinon operators act onto the spin effective lattice occupancies. The state representations of the new hidden global $U(1)$ symmetry are generated by the c fermion occupancy configurations in the c effective lattice. As mentioned above, the point is that for each energy eigenstate the relative positions of the sites of the η-spin and spin effective lattices in the original lattice are stored in the c effective lattice: For $U/4t > 0$ the latter lattice is identical to the original lattice for all $4^{N_a^2}$ energy eigenstates and the $N_c = 2S_c$ c fermions occupy the $2S_c$ sites singly occupied in the original lattice by the rotated electrons of the description introduced in Ref.[12]. We recall that for $U/4t > 0$ the sites of (i) the η-spin effective lattice and (ii) the spin effective lattice correspond to those (i) singly occupied and (ii) unoccupied and doubly occupied by rotated electrons. Hence for each energy eigenstate the relative positions of the sites of the (i) η-spin effective lattice and (ii) spin effective lattice in the original lattice refer to the relative positions of the sites of the c effective lattice (i) unoccupied by c fermions and (ii) occupied by c fermions, respectively.

That the relative positions of the sites of the η-spin and spin effective lattices in the original lattice are stored in the c fermion occupancy configurations of the c effective lattice is consistent with for $N_a^2 \rightarrow \infty$, $N^2_{a_\eta}/N_a^2 = [1 - 2S_c/N_a^2] > 0$, and $N^2_{a_s}/N_a^2 = 2S_c/N_a^2 > 0$ the occupancy configurations of the η-spinons and spinons of the general description of Ref.[12] referring to independent η-spin and spin effective lattices, respectively. Moreover, in that limit these lattices

can be considered as square lattices with spacing a_η and a_s, respectively, provided in Eq. (A8) of Appendix A. For the one- and two-electron subspace the latter spacing reads $a_s = a/\sqrt{1-x}$, as given in Eq. (18). Hence alike for $x = 0$ and $m = 0$ ground state, for $x > 0$ and $m = 0$ ground states the the $M_s = 2S_c$ spin-1/2 spinons remain occupying a full spin effective lattice with $N^2_{a_s} = M_s = 2S_c$ sites.

Although in the limit $N^2_a \rightarrow \infty$ the occupancies of the spin, η-spin, and c effective lattices are independent, for the $x > 0$ Hubbard model on the square lattice in the one- and two-electron subspace the $M_s = 2S_c$ spin-1/2 spinons interact with each other and with the c fermions. However, as mentioned above the expression of the $x > 0$ Hamiltonian (5) in the one- and two-electron subspace in terms of c fermion operators and spinon operators leads to a very involved quantum problem. Indeed, the usefulness of the c, spin, and $s1$ effective lattices and corresponding c and $s1$ momentum bands description refers to that Hamiltonian in the one- and two-electron subspace in normal order relative to the initial $x > 0$ and $m = 0$ ground state. Fortunately, such a ground-state normal-ordering simplifies the quantum problem[19]. It provides implicitly and naturally a criterion for the selection of a few dominant Hamiltonian terms expressed in terms of c fermion operators and two-spinon $s1$ fermion operators. That problem is studied in Ref.[19] in terms of a suitable energy functional valid for intermediate and large values of $U/4t$. The spin degrees of freedom of such a functional describe both the $x = 0$ and $x > 0$ problems. The model spin spectrum relative to the $x = 0$ and $m = 0$ ground state is one of the few problems for which there are results from controlled approximations involving summation of an infinite set of ladder diagrams[38]. As mentioned above, the spin spectrum provided by the energy functional of Ref.[19] quantitatively agrees with both the spin-wave spectrum derived in Ref.[38] and that observed in the parent compound LCO[3].

Alike for the $x = 0$ and $m = 0$ ground state, for $x > 0$ and $m = 0$ ground states the $M_s = 2S_c$ spinons remain confined within $N_{s1} = S_c$ spin-neutral two-spinon $s1$ fermions. The $s1$ fermions are generated from bosonic spin-neutral two-spinon $s1$ bond particles and thus have long-range interactions associated with the effective vector potential $\vec{A}_{s1}(\vec{r}_j)$ of Eq. (A2) of Appendix A. An important property is that for $x > 0$ and $m = 0$ ground states the $s1$ fermion momentum band is full and for one-electron and two-electron excited states displays a single hole and none or two holes, respectively[19]. The $s1$ - $s1$ fermion interactions associated with the effective vector potential of Eq. (A2) of Appendix A are stronger than those that arise between the emerging $s1$ fermions and pre-existing c fermions. In spite of that, the former do not lead to $s1$ - $s1$ fermion inelastic scattering. The obvious reason is that due to phase-space restrictions associated with the exclusion principle and energy and momentum conservation requirements there are no available momentum values in the $s1$ band for excited-state occupancy configurations.

Both for the $x = 0$ and $m = 0$ ground state and $x > 0$ and $m = 0$ ground states the $M_s = 2S_c$ spin-1/2 spinons occupy a full spin effective lattice with $N^2_{a_s} = M_s = 2S_c$ sites. However, an important point is that within the present description there is a qualitative difference between the $x = 0$ and $x > 0$ problems. At $x = 0$ the spin effective lattice is identical to the original lattice whereas for $x > 0$ it has a smaller number of sites $N^2_{a_s} = 2S_c < N^2_a$ so that its spacing $a_s = a/\sqrt{1-x}$ is larger. Within the description of the problem used in the studies of this paper, this is one of the main effects of hole doping. Indeed, the lack of the η-spin effective lattice, $N^2_{a_\eta} = x\, N^2_a = 0$, occurring at $x = 0$ implies that the spin effective lattice is identical to the original lattice and thus has the same number of sites $N^2_{a_s} = 2S_c = N^2_a$ as that lattice. We argue that the spin effective lattice being identical to the original lattice is a necessary condition for the ground-state long-range antiferromagnetic order to emerge as $N^2_a \rightarrow \infty$. The concepts of spin effective lattice and $s1$ effective lattice are only valid in that limit. Only in it are such lattices approximate square lattices with spacing $a_s = a/\sqrt{1-x}$ given in Eq. (18) and $a_{s1} \approx \sqrt{2}\, a_s$ provided in Eq. (21), respectively. The incommensurability relative to the original square lattice spacing a of the effective lattice spacings $a_s = a/\sqrt{1-x}$ and $a_{s1} \approx \sqrt{2}\, a_s$ is consistent with a ground-state long-range antiferromagnetic order occurring for $N^2_a \rightarrow \infty$ only at $x = 0$. Such an incommensurability allows processes that destroy long-range antiferromagnetic order becoming active for $x > 0$. Within the expansion in powers of t/U of the Hamiltonian (5), such processes are associated for instance with Hamiltonian terms with odd powers in t, absent at $x = 0$.

The possible existence of low-lying spin excitations for $x > 0$ is not a sufficient condition for a spontaneously broken symmetry to occur in the limit $N^2_a \rightarrow \infty$. According to the results of Ref.[12], the $m = 0$ and $x > 0$ ground states are for $N^2_a \gg 1$ large but finite spin-singlet states. Note though that only if the state obtained by application of the two-electron spin-flip operator onto such ground states had finite overlap with low-lying spin excitations would these states acquire a long-range spin order as $N^2_a \rightarrow \infty$. However, we argue that if low-lying spin excitations exist for $m = 0$ and $x > 0$ such an overlap vanishes. It vanishes as well in the case of non existence of low-lying spin excitations due to a spin gap: There is no coherent spin spectral weight both for vanishing and/or finite energy. Therefore, in addition to the $m = 0$ and $x > 0$ ground states remaining spin-singlet states in that limit, the corresponding spin-triplet spectrum is fully incoherent: Its sharp spectral features are not δ-function like. The absence of coherent spin-wave excitations is consistent with the lack of long-range spin order in the $m = 0$ and $x > 0$ ground states in the limit $N^2_a \rightarrow \infty$.

For a $x > 0$ and $m = 0$ ground state one has that the number of sites of the η-spin effective lattice $N^2_{a_\eta} = x\, N^2_a > 0$

is non zero even if the hole concentration $0 < x \ll 1$ is very small. For such a state the spin effective lattice has a number of sites $N_{a_s}^2 < N_a^2$ smaller than that of the original lattice. Consistently with the corresponding effective lattice spacings reading $a_s = a/\sqrt{1-x}$ and $a_{s1} \approx \sqrt{2}\, a_s$, below further evidence is provided that for $0 < x \ll 1$ the ground state of the Hubbard model on the square lattice has a short-range incomensurate-spiral spin order. Moreover, according to the results of Ref.[19] the ground state has a short-range spin order for $0 < x < x_*$. For $x > x_*$ it is a disordered state without short-range spin order. Here $x_* > 0.23$ for approximately $U/4t > u_0 \approx 1.3$.

Finally, we provide further evidence that the form of the $s1$ effective lattice spacing (21) is for the Hubbard model on the square-lattice consistent with the above mentioned $x = 0$ and $x > 0$ spin orders, respectively. That at $x = 0$ and $m = 0$ the spacing of the square $s1$ effective lattice is given by $a_{s1} = \sqrt{2}\, a$ reveals that then its periodicity has increased relative to that of the original lattice, which in that case is identical to the spin effective lattice. Indeed, at $x = 0$ the $s1$ effective lattice is one of the two sub-lattices of the original lattice and thus refers to a $\sqrt{2} \times \sqrt{2}$ reconstruction in which the periodicity of the spin-sub-system real-space structure is increased. Such an effect is consistent with the occurrence of the long-range antiferromagnetic order for $N_a^2 \rightarrow \infty$ at $x = 0$ and $m = 0$. In turn, that for $x > 0$ and $m = 0$ the square $s1$ effective lattice spacing reads instead $a_{s1} \approx \sqrt{2/(1-x)}\, a$ is consistent with the emergence of the short-range incommensurate-spiral spin order. Indeed now the $s1$ effective lattice is one of the two sub-lattices of the spin effective lattice which for $x > 0$ is different from and incommensurate to the original lattice.

2. Quantum and thermal phase transitions

It is argued above that the lack of finite overlap of the state generated by application of the two-electron spin-flip operator onto a $x > 0$ and $m = 0$ ground state with low-lying excited states is behind such a ground state remaining a spin-singlet state for $N_a^2 \rightarrow \infty$, alike for $N_a^2 \gg 1$ large but finite[12]. This is so independently of the existence or non existence (spin gap) of spin-triplet low-lying states. Hence such a ground state has no long-range antiferromagnetic order in the limit $N_a^2 \rightarrow \infty$ and its symmetry is that of the Hamiltonian, $SO(3) \times SO(3) \times U(1) = [SU(2) \times SU(2) \times U(1)]/Z_2^2$. A necessary condition for the occurrence of such a long-range order is according to our above analysis that the spin effective lattice is identical to the original lattice. That condition is not met by $x > 0$ and $m = 0$ ground states. For them the Hamiltonian hidden global $U(1)$ symmetry generator eigenvalue S_c obeys the inequality $S_c < N_a^2/2$. It then follows that the number of sites of the η-spin effective lattice $N_{a_\eta}^2 = [N_a^2 - 2S_c] > 0$ is finite, so that the number of sites of the spin effective lattice $N_{a_s}^2 = 2S_c < N_a^2$ is smaller than the number of sites of the original lattice. For the one- and two-electron subspace considered in this paper such inequalities read $N_{a_\eta}^2 = x\, N_a^2 > 0$ and $N_{a_s}^2 = (1-x)\, N_a^2 < N_a^2$, respectively.

There is strong evidence of the occurrence in the half-filled Hubbard model on the square lattice of strong short-range antiferromagnetic correlations for finite temperatures $T > 0$ below a crossover temperature called T_x in Ref.[29], which here we denote by T_0^*. This is consistent with then the system being driven into a phase with short-range spin order. Furthermore, that the occurrence of long-range antiferromagnetic order as $N_a^2 \rightarrow \infty$ requires that $T = 0$, $N_{a_\eta}^2 = 0$, and $N_{a_s}^2 = N_a^2$ is consistent with the short-range spin order occurring for $m = 0$, $0 < x \ll 1$, and $0 \leq T < T_0^*$ having basic similarities to that occurring for $m = 0$, $x = 0$, and $0 < T < T_0^*$. The latter order was studied previously in Ref.[29] for $0 < T \ll T_0^*$.

As further justified below, for both vanishing and finite temperatures a phase displaying a short-range spiral-incommensurate spin order is then expected to occur for (i) $m = 0$, $0 < x \ll 1$, and $0 \leq T \ll T_0^*$ and (ii) $m = 0$, $x = 0$, and $0 < T \ll T_0^*$. At $m = 0$ and temperatures below T_0^*, the system is driven both for (i) $0 < x \ll 1$ and $0 \leq T < T_0^*$ and (ii) $x = 0$ and $0 < T < T_0^*$ into a renormalized classical regime where the $N_a^2 \rightarrow \infty$, $x = 0$, and $T = 0$ long-range antiferromagnetic order is replaced by such a short-range spin order, which is a quasi-long-range spin order as that studied in Ref.[40] for simpler spin systems.

An interesting physical issue is whether the quantum phase transition separating the $x = 0$ and $m = 0$ ground state from the $0 < x \ll 1$ ground state at $T = 0$ corresponds to a "deconfined" quantum critical point[20]. Indeed, both at $x = 0$ and for $0 < x \ll 1$ the ground-state $M_s = 2S_c$ spinons are confined within $N_{s1} = S_c$ spin-neutral two-spinon $s1$ fermions. When expressed in terms of rotated-electron creation and annihilation operators, the Hamiltonian of the Hubbard model on the square lattice has for $U/4t$ finite an infinite number of terms, as given in Eq. (5). As mentioned above, the Hamiltonian terms generated up to fourth order in t/U are for $x > 0$ and within a unitary transformation the equivalent to the $t - J$ model with ring exchange and various correlated hoppings[13]. In addition to non-frustated isotropic spin interactions as those considered for a spin-1/2 Heisenberg model on the square lattice in Refs.[21,22], the present spinons have some degree of frustration as well. Hence their interactions cannot be studied by Quantum-Monte Carlo simulations due to the "sign problem". A related interesting open question is whether for $x > 0$ and $m = 0$ the the spin degrees of freedom of the present square-lattice quantum liquid refer to a valence-bond solid or some type of related valence-bond liquid. In either case, that both at $x = 0$ and for $x > 0$ the $M_s = 2S_c$

spinons are confined within $N_{s1} = S_c$ spin-neutral two-spinon $s1$ fermions strongly suggests that the corresponding quantum phase transition refers indeed to a "deconfined" quantum critical point. If this is so, the critical point is characterized by deconfined spin-1/2 spinons coupled to some emergent $U(1)$ gauge field[20–22].

We denote by $2\Delta_0$ the energy below which the short-range incommensurate-spiral spin order with strong antiferromagnetic correlations survives at zero-temperature, $m = 0$, and $0 < x \ll 1$. That energy parameter has a $U/4t$ dependence qualitatively similar to that of the energy scale $2k_B T_0^*$, with the equality $2\Delta_0 \approx 2k_B T_0^*$ approximately holding. Except for $U/4t \rightarrow 0$, such an energy scale has a different origin than the order parameter $\mu^0 = U\, m_{AF}\, \alpha^0$ of Eq. (43), which is proportional to the sub-lattice magnetization m_{AF} of Eq. (35). Indeed, for $0 < x \ll 1$ the lack of a long-range antiferromagnetic order implies that $m_{AF} = 0$.

3. *The $U/4t$ dependence of the $0 < x \ll 1$ energy scales*

The energy scale $2\Delta_0 \approx 2k_B T_0^*$ considered here plays a major role in the square-lattice quantum-liquid studies of Ref.[19]. Here we address the problem of its $U/4t$ dependence by combining the results obtained from the use of our general description with those of the low-temperature approach to the half-filled Hubbard model on the square lattice of Ref.[29]. The investigations of that reference focus on temperatures $0 < T \ll T_0^*$. The energy parameter $2\Delta_0 \approx 2k_B T_0^*$ refers to the limit $2\Delta_0 = \lim_{x\rightarrow 0} 2|\Delta|$ of an x dependent energy scale $2|\Delta|$ that plays the role of order parameter of the phase with short-range spin order. For $0 < x \ll 1$ and intermediate and large $U/4t$ values such an energy scale reads,

$$2|\Delta| \approx 2\Delta_0 \left(1 - \frac{x}{x_*^0}\right) , \quad 0 < x \ll 1 , \quad U/4t \geq u_0 \approx 1.302 . \tag{46}$$

The linear dependence on x of $[2\Delta_0 - 2|\Delta|] \approx (x/x_*^0)\, 2\Delta_0$ for $0 < x \ll 1$ is justified in Ref.[19]. Here $x_*^0 \approx 2r_s/\pi$, the ratio $r_s = 2\Delta_0/8W_{s1}^0$ plays an important role in the square-lattice quantum liquid, and $W_{s1}^0 \equiv \lim_{x\rightarrow 0} W_{s1} = W_{s1}|_{x=0}$ where W_{s1} is the nodal energy bandwidth W_{s1} of the $s1$ fermion dispersion defined in Ref.[19]. Its maximum magnitude is reached at $U/4t = 0$. For $U/4t > 0$ it decreases monotonously for increasing values of $U/4t$, vanishing for $U/4t \rightarrow \infty$. That for $U/4t \rightarrow \infty$ both $W_{s1} \rightarrow 0$ and $|\Delta| \rightarrow 0$ is associated with the full degeneracy of the spin configurations reached in that limit. In it the spectrum of the two-spinon composite $s1$ fermions becomes dispersionless. The limiting behaviors of the $m = 0$ energy parameter $8W_{s1}^0 \equiv \lim_{x\rightarrow 0} 8W_{s1} = 8W_{s1}|_{x=0}$ contributing to the ratio $r_s = 2\Delta_0/8W_{s1}^0$ read[19],

$$8W_{s1}^0 = 32t , \quad U/4t = 0 ; \qquad 8W_{s1}^0 \approx \frac{\pi}{2}\frac{[8t]^2}{U} , \quad U/8^2t \gg 1 . \tag{47}$$

In contrast to the $x > 0$ energy parameter $2|\Delta|$, the energy scale W_{s1}^0 is well defined both at $x = 0$ and for $x > 0$, having the same magnitude at $x = 0$ and for $x \rightarrow 0$. Its magnitude $W_{s1}^0(u_*) = [49.6/295]\, t \approx 0.168\, t$ obtained at $U/4t = u^* = 1.525$ in Ref.[19] is about 12.25 times smaller than that found by use of the limiting expression $4\pi\, t^2/U \approx 2.060\, t$ of Eq. (47) at $U/4t = 1.525$. This reveals that such a limiting expression is valid for a smaller range of very large $U/4t$ values than in 1D. Indeed, $4\pi\, t^2/U \approx 0.168\, t$ at $U/4t \approx 18.70$, whereas $W_{s1}^0 \approx 0.168\, t$ at $U/4t \approx 1.525$. Therefore, the relation $W_{s1}^0 = J \approx 4\pi\, t^2/U$ is valid for approximately $U/8^2t \gg 1$, as given in Eq. (47). For the Hubbard model on the square lattice the energy scale $J \approx 4\pi\, t^2/U$ controls the physics for a smaller $U/4t$ range than in 1D, which corresponds to very large $U/4t$ values such that $U/8^2t \gg 1$. Hence the intermediate-$U/4t$ range plays a major role in the physics of that model, as confirmed by the related studies of Ref.[19].

That for $U/4t > 0$ the energy scale $2\Delta_0 = \lim_{x\rightarrow 0} 2|\Delta|$ has a different origin than the order parameter $\mu^0 = U\, m_{AF}\, \alpha^0$ of Eq. (43) is consistent with for $U/4t > 0$ their magnitudes being different. However, symmetry arguments related to the disappearance of the $N_a^2 \rightarrow \infty$ and $x = 0$ ground-state long-range antiferromagnetic order for $U/4t \rightarrow 0$ imply that $\lim_{U/4t\rightarrow 0} 2\Delta_0 = \mu^0$. Indeed the ratio $2\Delta_0/\mu^0 \rightarrow 1$ involving the two energy scales becomes one in that limit. Moreover, the energy scale $2\Delta_0$ interpolates between $2\Delta_0 = \mu^0 \approx 32t\, e^{-\pi\sqrt{4t/U}}$ for $U/4t \ll 1$ and $2\Delta_0 = 8W_{s1}^0 \approx \pi\,[8t]^2/U$ for approximately $U/8^2t \gg 1$. It goes through a maximum magnitude at a $U/4t$ value found below to be approximately given by $U/4t = u_0 \approx 1.302$.

The energy parameter μ_0 is an increasing function of $U/4t$. As given in Eq. (42), it behaves as $\mu_0 \approx 32\, t\, e^{-\pi\sqrt{\frac{4t}{U}}}$ for $U/4t \ll 1$ and as $\mu_0 \approx [U - 8t]$ for $U/4t \gg 1$. In turn, the energy scale $8W_{s1}^0$ is a decreasing function of $U/4t$. According to Eq. (47) it is given by $8W_{s1}^0 = 32t$ at $U/4t = 0$ and decreases approximately as $8W_{s1}^0 \approx \pi\,[8t]^2/U$ for very large $U/4t$. Since the energy scale $2\Delta_0$ interpolates between these two behaviors, it vanishes both for $U/4t \rightarrow 0$ and $U/4t \rightarrow \infty$ as $2\Delta_0 \approx 32t\, e^{-\pi\sqrt{4t/U}}$ and $2\Delta_0 \approx \pi(8t)^2/U$, respectively. In these two limits it becomes μ_0 and the energy scale $8W_{s1}^0 \approx \pi(8t)^2/U$ associated with the strong $0 < x \ll 1$ antiferromagnetic correlations, respectively.

This is consistent with its maximum magnitude being reached at an intermediate $U/4t$ value $U/4t = u_0$ at which the equality $\mu_0 \approx 8W^0_{s1}$ holds. We then define such a $U/4t$ value as that at which the lines $8W^0_{s1} = 8W^0_{s1}(U/4t)$ and $\mu_0 = \mu_0(U/4t)$ cross and thus the equality $\mu_0(u_0) = 8W^0_{s1}(u_0)$ holds. The ratio $r_s = 2\Delta_0/8W^0_{s1}$ is parametrized in the following as $r_s = e^{-\lambda_s}$ where $\lambda_s = |\ln(2\Delta_0/8W^0_{s1})|$ controls such an interpolation behavior.

The energy scale $2\Delta_0$ can then be expressed as,

$$2\Delta_0 = r_s\, 8W^0_{s1} = 8W^0_{s1}\, e^{-\lambda_s}\,; \quad \lambda_s = |\ln(2\Delta_0/8W^0_{s1})|\,, \tag{48}$$

where λ_s has the limiting behaviors,

$$\begin{aligned} \lambda_s &= \pi\sqrt{4t/U}\,, \quad U/4t \ll 1\,; \qquad \lambda_s \approx 4t\,u_0/U\,, \quad u_{00} \le U/4t \le u_1\,; \qquad \lambda_s = 0\,, \quad U/4t \to \infty\,, \\ u_{00} &\approx (u_0/\pi)^2 \approx 0.171\,; \quad u_0 \approx 1.302\,; \quad u_1 \approx 1.600\,. \end{aligned} \tag{49}$$

The ratio $r_s = 2\Delta_0/8W^0_{s1}$ is an increasing function of $U/4t$. It changes continuously from $r_s = 0$ for $U/4t \to 0$ to $r_s = 1$ for $U/4t \to \infty$. For $u_{00} \le U/4t \le u_1$ it is approximately given by $r_s \approx e^{-4t\,u_0/U}$ rather than by $r_s \approx e^{-\pi\sqrt{4t/U}}$ for $U/4t \ll 1$. This is consistent with for large $U/4t$ values $(1 - r_s)$ being proportional to $(1 - r_s) \propto 4t/U$ rather than to $(1 - r_s) \propto \sqrt{4t/U}$.

The temperature T_x of Ref.[29] that plays the role of our temperature $T^*_0 \approx 2\Delta_0/2k_B$ is plotted in Fig. 3 of that reference. Its $U/4t$ dependence is qualitatively correct. T_x vanishes both in the limits $U/4t \to 0$ and $U/4t \to \infty$. It goes through a maximum magnitude at an intermediate value $5/4 < U/4t < 3/2$. Nevertheless, the interpolation function used to produce it, provided in Ref. 74 of such a paper, is poor for intermediate values of $U/4t$. However, that does not affect the validity of the results of Ref.[29]. Indeed, the studies of that reference refer to the temperature range $0 < T \ll T_x$ for which the accurate dependence of T_x on $U/4t$ is not needed. The goal of its Fig. 3 is merely illustrating qualitatively the T_x behavior over the entire coupling range[41].

The studies of Ref.[19] on the square-lattice quantum liquid refer mostly to intermediate $U/4t$ values. Given the important role plaid by the energy scale $2\Delta_0 \approx 2k_B\,T^*_0$ in the physics of that quantum liquid, we need a more quantitatively accurate $U/4t$ dependence of it for intermediate $U/4t$ values. Such a dependence must be consistent with the qualitative physical picture of Ref.[29]. According to Eqs. (48) and (49) one has that $2\Delta_0 = 8W^0_{s1}\, e^{-\lambda_s}$ for $U/4t > 0$. Here the parameter λ_s is a continuous decreasing function of $U/4t$. It is given by $\lambda_s = \infty$ for $U/4t \to 0$ and $\lambda_s = 0$ for $U/4t \to \infty$. This reveals that the magnitude $\lambda_s = 1$ separates two physical regimes. Consistently, $\lambda_s = 1$ refers to the $U/4t$ value $U/4t = u_0$ at which $2\Delta_0$ reaches its maximum magnitude, $\max\{2\Delta_0\} = [\mu_0(u_0)]\, e^{-1} = 8W^0_{s1}(u_0)\, e^{-1}$.

That as found in Ref.[19] the parameter x^0_* is for approximately $u_0 \le U/4t \le u_1$ given by $x^0_* = 2r_s/\pi = 2e^{-4t\,u_0/U}/\pi$ and at $U/4t \approx u_* = 1.525$ reads $x^0_* \approx 0.27$ implies that $u_0 \approx 1.3$. Moreover, in that reference it is found that $8W^0_{s1}(u_*) = [396.8/295]\, t \approx 1.345\, t$ at $U/4t \approx u_* = 1.525$. Such a result is obtained in that reference from comparison of the $x = 0$ and $m = 0$ spin excitation spectra for the high symmetry directions found by use of the c and $s1$ fermion description with those estimated by the controlled approximation of Ref.[38]. On combining the equality $\mu_0(u_0) = 8W^0_{s1}(u_0)$ with the magnitude $\mu_0(u_0) \approx [2e^1/\pi]\, t$ of Eq. (42) we find $8W^0_{s1}(u_0) \approx [2e^1/\pi]\, t \approx 1.731\, t$ and $\max\{2\Delta_0\} = [\mu_0(u_0)]\, e^{-1} = 8W^0_{s1}(u_0)\, e^{-1} \approx 2t/\pi$.

For the intermediate range $U/4t \in (u_0, u_1)$ the $U/4t$ dependence of the energy parameter $8W^0_{s1}$ is of the form $8W^0_{s1} \approx [2e^1/\pi]\, t\, W(U/4t)$. Here $W(u)$ is an unknown function of $u = U/4t$ such that $W(u_0) = 1$. On combining Eqs. (48) and (49) one finds $2\Delta_0 = 8W^0_{s1}\, e^{-4t\,u_0/U}$. Thus fulfillment of the maximum condition $\partial 2\Delta_0(u)/\partial u = 0$ at $u = u/4t = u_0$ requires the function $W(u)$ be given by $W(u) \approx (2 - u/u_0)$ for $0 \le [(u - u_0)/(u_1 - u_0)] \ll 1$. In turn, the use of the above results $8W^0_{s1}(u_*) = [396.8/295]\, t \approx 1.345\, t$ and $8W^0_{s1}(u_0) \approx [2e^1/\pi]\, t \approx 1.731\, t$ reveals that the ratio $8W^0_{s1}(u_*)/8W^0_{s1}(u_0)$ may be expressed as $8W^0_{s1}(u_*)/8W^0_{s1}(u_0) \approx [1 - (u_* - u_0)]$. It then follows that $W(u) \approx [1 - (u - u_0)]$ for $u \approx u_* = 1.525$. We then use a suitable interpolation function for $W(u)$, which has these two limiting behaviors. The energy parameter $8W^0_{s1}$ is for $U/4t$ intermediate values $U/4t \in (u_0, u_1)$ then given approximately by,

$$\begin{aligned} 8W^0_{s1} &\approx \frac{2e^1\, t}{\pi}\, W(U/4t)\,; \quad W(u) \approx 1 - (u - u_0)\, e^{-\frac{u_* - u}{u_* - u_0}\ln(u_0)}\,, \quad u_0 \le U/4t \le u_1\,, \\ u_0 &\approx u_* - 1 + e^{-1}\pi\frac{198.4}{295} \approx 1.302\,; \quad u_* \approx 1.525\,. \end{aligned} \tag{50}$$

The value $u_0 \approx 1.302$ is that obtained from the equation $8W^0_{s1}(u_*) = [2e^1\, t/\pi]\, [1 - (u_* - u_0)] = [396.8/295]\, t \approx 1.731\, t$.

On combining the above results we find the following approximate behaviors for the energy parameter $2\Delta_0$,

$$\begin{aligned} 2\Delta_0 &\approx 32t\, e^{-\pi\sqrt{4t/U}}\,, \quad U/4t \ll 1\,, \\ &= \max\{2\Delta_0\} \approx 2t/\pi\,, \quad U/4t = u_0\,, \\ &\approx e^{(1-4t\,u_0/U)}[2t/\pi]\, W(U/4t)\,, \quad u_0 \le U/4t \le u_1\,, \\ &= 8W^0_{s1} \approx [\pi\,(8t)^2/2U]\,, \quad U/8^2t \gg 1\,. \end{aligned} \tag{51}$$

Here $W(U/4t)$ is the interpolation function given in Eq. (50). Note that $\partial 2\Delta_0(u)/\partial u = 0$ at $u = u/4t = u_0$, consistently with $2\Delta_0$ reaching its maximum magnitude $2t/\pi$ at that $U/4t$ value. The overall U/t dependence of $T_0^* \approx 2\Delta_0/2k_B$ is similar to that plotted in Fig. 3 of Ref.[29] for T_x with the U/t value at which the maximum magnitude is reached shifted from $U/t \approx 5.60$ to $U/t \approx 5.21$. Moreover, that magnitude is lessened from $\max\{T_x\} \approx 0.625\, t/k_B$ to $\max\{T_0^*\} \approx \max\{2\Delta_0/2k_B\} \approx t/[\pi k_B] \approx 0.318\, t/k_B$.

4. *Short-range incommensurate spiral spin order for* $0 < x \ll 1$ *and* $T = 0$

Here we provide strong evidence that for intermediate and large values of $U/4t$ and small hole concentrations $0 < x \ll 1$ the short-range spin order of the $m = 0$ ground state corresponds indeed to that of a spin-singlet incommensurate spiral state. In terms of the rotated-electron spins occupancy configurations the ground state is then a spin-singlet incommensurate spiral state for $U/4t > 0$, $m = 0$, and $0 < x \ll 1$. That evidence is found on combining several results. This includes the necessary condition for occurrence of a long-range spin order for $N_a^2 \rightarrow \infty$ argued in Section III-C to be that the spin effective lattice is identical to the original lattice and thus $N_{a_s}^2 = 2S_c = N_a^2$, the result of Ref.[12] that the $m = 0$ and $0 < x \ll 1$ ground state is a spin-singlet state for $N_a^2 \gg 1$ and thus remains so for $N_a^2 \rightarrow \infty$, and the results of Ref.[34] concerning the spin degrees of freedom of a related quantum problem.

As discussed in Section I, for intermediate and large values of $U/4t$ the Hubbard model on the square lattice given in Eqs. (1) and (5) in terms of electron and rotated-electron operators, respectively, can be mapped onto an effective $t-J$ model on a square lattice with t, $t' = t'(U/4t)$, and $t'' = t''(U/4t)$ transfer integrals. The role of the processes associated with $t' = t'(U/4t)$ and $t'' = t''(U/4t)$ becomes increasingly important upon decreasing the $U/4t$ value. Reference[34] presents rigorous results on the spin degrees of freedom of the $t-J$ model on a square lattice with t, t', and t'' transfer integrals. The investigations of that paper refer to small values of the hole concentration $0 < x \ll 1$ and spin density $m = 0$. Their starting point is a suitable action first introduced in Ref.[42]. The use in Ref.[34] of a staggered CP^1 representation for the spin degrees of freedom allows to resolve exactly the constraint against double occupancy. Within our description of the problem, this is is equivalent to performing the electron - rotated-electron unitary transformation. In order to achieve the rigorous result that for small hole concentrations there occurs a incommensurate-spiral spin order, the effective action for the spin degrees of freedom is reached after integrating out the charge fermionic degrees of freedom and the magnetic fast CP^1 modes. Importantly, the dependence on the hole concentration of the coupling constants of the effective field theory is in Ref.[34] obtained explicitly for small x.

We consider the mapping between the above effective $t-J$ model and the Hubbard model of Eqs. (1) and (5) in the subspace with vanishing rotated-electron double-occupancy. Accounting for such a mapping, the studies of Ref.[34] imply that for intermediate and large values of $U/4t$, spin-density $m = 0$, and small hole concentrations $0 < x \ll 1$ the ground state of the Hubbard model on the square lattice is an incommensurate spiral state. This is a rigorous result. However the studies of Ref.[34] are not conclusive on whether for $N_a^2 \rightarrow \infty$ and $0 < x \ll 1$ the $m = 0$ incommensurate spiral ground state has short-range or long-range spin order.

The necessary condition for occurrence in the limit $N_a^2 \rightarrow \infty$ of a ground-state long-range spin order argued in Section III-C to be that the spin effective lattice is identical to the original lattice and thus $N_{a_s}^2 = 2S_c = N_a^2$ is not fulfilled for $0 < x \ll 1$. We thus argue that in the thermodynamic limit $N_a^2 \rightarrow \infty$ the $0 < x \ll 1$ and $m = 0$ incommensurate spiral ground state has no long-range spin order. Hence such a ground state has the same symmetry and basic properties both for $N_a^2 \gg 1$ very large but finite and for $N_a^2 \rightarrow \infty$. One then combines the result of Ref.[12] that for $N_a^2 \gg 1$ and thus for $N_a^2 \rightarrow \infty$ the $m = 0$ and $0 < x \ll 1$ ground state of the Hubbard model on the square lattice (1) is a spin-singlet state with that of Ref.[34] that it is a incommensurate spiral state. This consistently implies that for $N_a^2 \rightarrow \infty$ and intermediate and large values of $U/4t$ the $m = 0$ and $0 < x \ll 1$ ground state of the Hubbard model on the square lattice is a spin-singlet state with short-range incommensurate-spiral spin order and strong antiferromagnetic correlations.

Finally, a ground-state short-range spin order does not preclude the occurrence of a ground-state long-range dimer-dimer order, as in a valence-bond solid. However, whether the spin degrees of freedom of the square-lattice quantum liquid refer for $x > 0$ and $m = 0$ to a valence-bond solid or a valence-bond liquid remains an open issue.

IV. CONCLUDING REMARKS

In this paper we considered a suitable one- and two-electron subspace in which the general operator description for the Hubbard model on a square lattice with $N_a^2 \gg 1$ sites introduced in Ref.[12] simplifies. When acting onto such a subspace the model refers to a two-component quantum liquid described in terms of charge c fermions and spin-neutral two-spinon $s1$ fermions. The one- and two-electron subspace can be divided into smaller subspaces that conserve S_c and S_s. Those are spanned by energy eigenstates whose generators have simple form in terms of c and

$s1$ fermion operators, as given in Eqs. (28) and (29). When expressed in terms of c and $s1$ fermion operators, the Hubbard model on a square lattice in the one- and two-electron subspace is the square-lattice quantum liquid further studied in Ref.[19]. That in such a subspace the c and $s1$ fermion momentum values are good quantum numbers plays a key role in the investigations of that reference. The one- and two-electron subspace considered in this paper contains nearly the whole spectral weight generated from application of one- and two-electron operators onto the exact ground state.

There is a large consensus that in the thermodynamic limit $N_a^2 \rightarrow \infty$ long-range antiferromagnetic order sets in in the $m = 0$ ground state of the half-filled Hubbard model on the square lattice[11,26–30]. Consistently, in this paper strong evidence is found that provided that in the thermodynamic limit $N_a^2 \rightarrow \infty$ a long-range antiferromagnetic order occurs in the ground state of the related isotropic spin-1/2 Heisenberg model on the square lattice, a similar long range order sets in in that limit in the ground state of the half-filled Hubbard model on the square lattice for $U/4t > 0$. Our results indicate that for $U/4t > 0$ a ground-state spontaneous symmetry breaking from $SO(3) \times SO(3) \times U(1)$ for large but finite number of lattice sites $N_a^2 \gg 1$ to $[U(2) \times U(1)]/Z_2^2 = [SO(3) \times U(1) \times U(1)]/Z_2$ in the thermodynamic limit $N_a^2 \rightarrow \infty$ occurs at $x = 0$ and $m = 0$ due to emergence of such a long-range antiferromagnetic order. Our analysis of the problem profits from the description of the ground states and low-lying energy eigenstates and corresponding state representations of the group $SO(3) \times SO(3) \times U(1)$ in terms of occupancy configurations of three effective lattices. Our results indicate that the spin effective lattice being identical to the original lattice and thus $N_{a_s}^2 = N_a^2$ is a necessary condition for the occurrence of a ground-state long-range antiferromagnetic order as $N_a^2 \rightarrow \infty$. The picture which emerges for $N_a^2 \rightarrow \infty$ is that of a ground state with long-range antiferromagnetic order for half filling and a short-range incommensurate-spiral spin order for $0 < x \ll 1$ and thus $N_{a_s}^2 < N_a^2$.

An interesting issue is whether the quantum phase transition separating the $x = 0$ and $m = 0$ ground state from the $0 < x \ll 1$ ground state at $T = 0$ corresponds to a "deconfined" quantum critical point[20–22]. That both at $x = 0$ and for $x > 0$ the $M_s = 2S_c$ spinons are confined within $N_{s1} = S_c$ spin-neutral two-spinon $s1$ fermions strongly suggests so. This would imply that the critical point is characterized by deconfined spin-1/2 spinons coupled to some emergent $U(1)$ gauge field. Furthermore, in this paper the general rotated-electron description behind the c and $s1$ fermion operator representation was also used to provide evidence that the Mermin and Wagner Theorem may apply at half-filling to all values $U/4t > 0$ of the Hubbard model on the square lattice.

The energy order parameters $\mu^0 = U\, m_{AF}\, \alpha^0$ of Eq. (43) and $2|\Delta|$ of Eq. (46) have a different physical origin. The energy scale μ^0 can be used as order parameter of the $T = 0$, $x = 0$, and $m = 0$ phase with long-range antiferromagnetic order. Indeed, it is proportional to the $x = 0$ and $m = 0$ sub-lattice magnetization m_{AF} of Eq. (35), which vanishes for $x > 0$. In turn, the energy order parameter $2|\Delta|$ is associated with the $x > 0$ and $m = 0$ short-range spin correlations. However, both μ^0 and $2|\Delta|$ are at $x = 0$ and for $x > 0$, respectively, identified in the studies of Ref.[19] with the maximum pairing energy of the $-1/2$ and $+1/2$ spinons of a composite spin-neutral two-spinon $s1$ fermion. The results of that reference extend the $m = 0$ and $T = 0$ short-range spin order found in this paper for $0 < x \ll 1$ to a well-defined range of hole concentrations $0 < x < x_*$. According to these results, the x dependence $2|\Delta| \approx 2\Delta_0(1 - x/x_*^0)$ given in Eq. (46) for $0 < x \ll 1$ is valid for $x \in (0, x_*)$. This holds provided that approximately $U/4t \in (u_0, u_\pi)$. Here $u_\pi > u_1$ where $u_1 \approx 1.6$ is the $U/4t$ value at which $r_s = 1/2$. For that $U/4t$ range the critical hole concentration x_* equals the $U/4t$-dependent parameter $x_*^0 = 2r_s/\pi$. The studies of Ref.[19] identify it with a critical hole concentration $x_* \equiv x_*^0$ above which there is no short-range spin order at $T = 0$. For $x > x_*$ and $T = 0$ a spin disordered state without short-range order for which the energy scale $2|\Delta|$ vanishes emerges. Consistently, $2|\Delta| \rightarrow 0$ as $0 < (x_* - x) \rightarrow 0$. The short-range incommensurate-spiral spin order discussed here for $0 < x \ll 1$ corresponds then to a limiting case of the general short-range spin order that according to the investigations of Ref.[19] occurs for $0 < x < x_*$ and approximately $U/4t \in (u_0, u_\pi)$. (That order occurs as well for $U/4t > u_\pi$, yet then the critical hole concentration x_* may not be given by $x_*^0 = 2r_s/\pi$.)

As confirmed in that reference, for the square-lattice quantum liquid introduced in this paper the c and $s1$ fermions play the role of "quasiparticles". There are three main differences relative to an isotropic Fermi liquid[43]. First, concerning the charge degrees of freedom, the non-interacting limit of the theory refers to $4t^2/U \rightarrow 0$ rather than to the limit of zero interaction $U \rightarrow 0$. Second, in the $4t^2/U \rightarrow 0$ limit the c fermions and $s1$ fermions become the holes of the "quasicharges" of Ref.[36] and spin-singlet two-spin configurations of the spins of such a reference rather than electrons. Indeed, only the charge dynamical structure factor becomes that of non-interacting spinless fermions. In turn, the one-electron and spin spectral distributions remain non-trivial. Third, for $U/4t > 0$ the $s1$ band is full for initial $m = 0$ ground states and displays a single hole for their one-electron excited states. As found in Ref.[19] its boundary line is anisotropic, what is behind anomalous one-electron scattering properties. Those involve the inelastic scattering of c fermions with momenta near the isotropic c Fermi line with $s1$ fermions with momenta in the vicinity of the anisotropic boundary line.

Concerning the relation to previous results on the Hubbard model on the square lattice and related models by other authors, as discussed above in this paper our results are consistent with and complementary to those of Refs.[29,30,34,36,38]. Elsewhere evidence is provided that upon addition of a weak three-dimensional uniaxial anisotropy

perturbation to the square-lattice quantum liquid, its short-range spin order coexists for $N_a^2 \rightarrow \infty$, low temperatures, and a well-defined range of hole concentrations with a long-range superconducting order.

Acknowledgments

I thank Daniel Arovas, Nicolas Dupuis, Alejandro Muramatsu, Stellan Östlund, Karlo Penc, Pedro D. Sacramento, and Maria Sampaio for discussions and the support of the ESF Science Program INSTANS and grant PTDC/FIS/64926/2006.

Appendix A: Results on the c fermion and $s1$ bond-particle description needed for our studies

For the LWS subspace defined in Ref.[12] the rotated-electron operators of Eq. (3) can be expressed in terms of the c fermion operators of real-space coordinate $\vec{r}_j$ and rotated quasi-spin operators $q^{\pm}_{\vec{r}_j} = s^{\pm}_{\vec{r}_j} + p^{\pm}_{\vec{r}_j}$ and $q^{x_3}_{\vec{r}_j} = s^{x_3}_{\vec{r}_j} + p^{x_3}_{\vec{r}_j}$ and thus of spinon operators $s^{\pm}_{\vec{r}_j}$ and $s^{x_3}_{\vec{r}_j}$ and η-spinon operators $p^{\pm}_{\vec{r}_j}$ and $p^{x_3}_{\vec{r}_j}$. This is achieved by inverting the relations given in Eqs. (6) and (9) with the result,

$$\tilde{c}^{\dagger}_{\vec{r}_j,\uparrow} = f^{\dagger}_{\vec{r}_j,c}\left(\frac{1}{2} + s^{x_3}_{\vec{r}_j} + p^{x_3}_{\vec{r}_j}\right) + e^{i\vec{\pi}\cdot\vec{r}_j}\, f_{\vec{r}_j,c}\left(\frac{1}{2} - s^{x_3}_{\vec{r}_j} - p^{x_3}_{\vec{r}_j}\right) \; ; \quad \tilde{c}^{\dagger}_{\vec{r}_j,\downarrow} = (s^{-}_{\vec{r}_j} + p^{-}_{\vec{r}_j})\,(f^{\dagger}_{\vec{r}_j,c} - e^{i\vec{\pi}\cdot\vec{r}_j}\, f_{\vec{r}_j,c})\,. \tag{A1}$$

The corresponding expressions of the rotated-electron annihilation operators are trivially obtained from those provided here.

As given in Eq. (6), Fourier transform of the c fermion operators $f^{\dagger}_{\vec{r}_j,c}$ generates the corresponding momentum c fermion operators $f^{\dagger}_{\vec{q}_j,c}$. Here the discrete momenta $\vec{q}_j$ are good quantum numbers[12]. In turn, the operators $f^{\dagger}_{\vec{q}_j,\alpha\nu}$ of the $\alpha\nu$ fermions also introduced in Ref.[12] act onto subspaces with constant values for the set of numbers S_α, $N_{\alpha\nu}$, and $\{N_{\alpha\nu'}\}$ for $\nu' > \nu$ and equivalently of the numbers S_c, $N_{\alpha\nu}$, and $\{N_{\alpha\nu'}\}$ for all $\nu' \neq \nu$. Here $\nu = 1, ..., C_\alpha$ is the number of η-spinon ($\alpha = \eta$) and spinon ($\alpha = s$) pairs confined within a composite $\alpha\nu$ fermion and the maximum ν value C_α is expressed below in Eq. (A5) in terms of $\alpha\nu$ fermion numbers $N_{\alpha\nu}$. The above subspaces are spanned by mutually neutral states, that is states with constant values for the numbers of $\alpha\nu$ fermions and $\alpha\nu$ fermion holes. Hence such states can be transformed into each other by $\alpha\nu$ band particle-hole processes. As a result of the transformation that maps the $\alpha\nu$ bond particles into $\alpha\nu$ fermions and provided that in the thermodynamic limit $N_a^2 \rightarrow \infty$ the ratio $N_{\alpha\nu}/N_a^2$ is finite for the $\alpha\nu$ branch under consideration, the latter composite fermions have long-range interactions associated with an effective vector potential $\vec{A}_{\alpha\nu}(\vec{r}_j)$[12,33,44]. For the one- and two-electron subspace considered in this paper the ratio $N_{\alpha\nu}/N_a^2$ remains finite in the limit $N_a^2 \rightarrow \infty$ only for the $s1$ fermion branch. For it the effective vector potential $\vec{A}_{s1}(\vec{r}_j)$ reads[12],

$$\begin{aligned}
\vec{A}_{s1}(\vec{r}_j) &= \Phi_0 \sum_{j' \neq j} n_{\vec{r}_{j'},s1}\, \frac{\vec{e}_{x_3} \times (\vec{r}_{j'} - \vec{r}_j)}{(\vec{r}_{j'} - \vec{r}_j)^2} \; ; \quad n_{\vec{r}_j,s1} = f^{\dagger}_{\vec{r}_j,s1}\, f_{\vec{r}_j,s1}\,, \\
\vec{B}_{s1}(\vec{r}_j) &= \vec{\nabla}_{\vec{r}_j} \times \vec{A}_{s1}(\vec{r}_j) = \Phi_0 \sum_{j' \neq j} n_{\vec{r}_{j'},s1}\, \delta(\vec{r}_{j'} - \vec{r}_j)\, \vec{e}_{x_3} \; ; \quad \Phi_0 = 1\,.
\end{aligned} \tag{A2}$$

Here $\vec{B}_{s1}$ is the corresponding fictitious magnetic field, $\vec{e}_{x_3}$ is the unit vector perpendicular to the plane, and we use units such that the fictitious magnetic flux quantum is given by $\Phi_0 = 1$. It follows from the form of the effective vector potential $\vec{A}_{s1}(\vec{r}_j)$ that the present description leads to the intriguing situation where the $s1$ fermions interact via long-range forces while all interactions in the original Hamiltonian are onsite.

The theory associated with the operator description introduced in Ref.[12] for the Hubbard model on the square lattice refers to a well-defined vacuum. For hole concentrations $0 \leq x < 1$ and maximum spin density $m = (1 - x)$ reached at a critical magnetic field H_c parallel to the square-lattice plane the c fermion operators are invariant under the electron - rotated-electron unitary transformation. Then there is a fully polarized vacuum $|0_{\eta s}\rangle$, which remains invariant under such a transformation. It reads,

$$|0_{\eta s}\rangle = |0_\eta; N^2_{a_\eta}\rangle \times |0_s; N^2_{a_s}\rangle \times |GS_c; 2S_c\rangle\,. \tag{A3}$$

Here the η-spin $SU(2)$ vacuum $|0_\eta; N^2_{a_\eta}\rangle$ associated with $N^2_{a_\eta}$ independent $+1/2$ η-spinons, the spin $SU(2)$ vacuum $|0_s; N^2_{a_s}\rangle$ with $N^2_{a_s}$ independent $+1/2$ spinons, and the c $U(1)$ vacuum $|GS_c; 2S_c\rangle$ with $N_c = 2S_c$ c fermions remain

invariant under the electron - rotated-electron unitary transformation. The explicit expression of the state $|GS_c;2S_c\rangle$ of Eq. (A3) in terms of the vacuum $|GS_c;0\rangle$ appearing in Eq. (29) is $\prod_{\vec{q}} f^{\dagger}_{\vec{q},c}|GS_c;0\rangle$. The vacuum $|GS_c;0\rangle$ is part of the electron and rotated-electron vacuum. The form of the latter vacuum is given by Eq. (A3) with $N^2_{a_\eta} = N^2_a$, $N^2_{a_s} = 2S_c = 0$, and thus $|GS_c;2S_c\rangle$ replaced by $|GS_c;0\rangle$. Only for a $m = (1-x)$ fully polarized state are the state $|GS_c;2S_c\rangle$ and the corresponding $N_c = 2S_c$ fermions invariant under the electron - rotated-electron unitary transformation for $U/4t > 0$.

The $\alpha\nu$ momentum band of the operators $f^{\dagger}_{\vec{q}_j,\alpha\nu}$ is associated with a well-defined $\alpha\nu$ effective lattice. The number $N^2_{a_{\alpha\nu}}$ of the $\alpha\nu$ band discrete momentum values exactly equals the number of sites of such an effective lattice. It is given by,

$$N^2_{a_{\alpha\nu}} = [N_{\alpha\nu} + N^h_{\alpha\nu}]\,, \tag{A4}$$

where the number of unoccupied sites reads,

$$N^h_{\alpha\nu} = [2S_\alpha + 2\sum_{\nu'=\nu+1}^{C_\alpha}(\nu'-\nu)N_{\alpha\nu'}] = [N^2_{a_\alpha} - \sum_{\nu'=1}^{C_\alpha}(\nu+\nu'-|\nu-\nu'|)N_{\alpha\nu'}]\,; \quad C_\alpha = \sum_{\nu=1}^{C_\alpha}\nu\,N_{\alpha\nu}\,. \tag{A5}$$

For the particular case of $\nu = 1$ the expression (A5) of the number of unoccupied sites of the $\alpha 1$ effective lattices simplifies to,

$$N^h_{\alpha 1} = [N^2_{a_\alpha} - 2B_\alpha]\,; \quad B_\alpha = \sum_{\nu=1}^{C_\alpha} N_{\alpha\nu}\,; \quad \alpha = \eta\,, s\,. \tag{A6}$$

This number equals that of $\alpha 1$ fermion holes in the $\alpha 1$ band.

According to the results of Ref.[12], all sites of the $s1$ effective lattice of $x > 0$ and $m = 0$ ground states are occupied and hence there are no unoccupied sites. In turn, the dominant contributions to the one-electron and two-electron excitations involve states with one and none or two unoccupied sites, respectively. For the square-lattice quantum liquid the expression of the related conserved number P^h_{s1} introduced in that reference simplifies to,

$$P^h_{s1} \equiv e^{i\pi N^h_{s1}} = e^{i2\pi S_s} = e^{i2\pi S_c} = e^{i\pi N} = \pm 1\,. \tag{A7}$$

Here N denotes the number of electrons. For the Hubbard model on the square lattice in the one- and two-electron subspace considered in this paper the number N^h_{s1} of unoccupied $s1$ effective lattice sites and thus of $s1$ fermion holes in the $s1$ momentum band is a good quantum number.

As discussed in Ref.[12], the η-spinon, spinon, and c fermion description contains full information about the relative positions of the sites of the η-spin and spin effective lattices in the original lattice. Hence it turns out that within the $N^2_a \gg 1$ limit and for finite values of the hole concentration x (and electron density $n = (1-x)$) the η-spin (and spin) effective lattice can be represented by a square lattice with spacing a_η (and a_s) given by,

$$a_\alpha = \frac{L}{N_{a_\alpha}} = \frac{N_a}{N_{a_\alpha}}\,a\,; \quad \alpha = \eta\,, s\,. \tag{A8}$$

Moreover, provided that in the thermodynamic limit $N^2_a \rightarrow \infty$ the ratio $N_{\alpha\nu}/N^2_a$ is finite, the related $\alpha\nu$ effective lattices can be represented by square lattices with spacing,

$$a_{\alpha\nu} = \frac{L}{N_{a_{\alpha\nu}}} = \frac{N_a}{N_{a_{\alpha\nu}}}\,a = \frac{N_{a_\alpha}}{N_{a_{\alpha\nu}}}\,a_\alpha\,; \quad N_{a_{\alpha\nu}} \geq 1\,, \tag{A9}$$

where $\nu = 1,...,C_\alpha$ and $\alpha = \eta, s$. In turn, the corresponding $\alpha\nu$ bands whose number of discrete momentum values is also given by $N^2_{a_{\alpha\nu}}$ are well defined even when $N^2_{a_{\alpha\nu}}$ is given by a finite small number, $N^2_{a_{\alpha\nu}} = 1, 2, 3, ...$

Finally, an important and useful property found in Ref.[12] is that the $\eta\nu$ fermions with any number $\nu = 1,...,C_\eta$ of η-spinon pairs and $s\nu$ fermions with $\nu = 2,...,C_s$ spinon pairs whose energy is given by,

$$\epsilon_{\eta\nu} = 2\nu\mu\,, \quad \nu = 1,...,C_\eta\,; \qquad \epsilon_{s\nu} = 2\nu\mu_B\,H\,, \quad \nu = 2,...,C_s\,, \tag{A10}$$

remain invariant under the electron - rotated-electron unitary transformation. Here H denotes the magnitude of a magnetic field aligned parallel to the square-lattice plane. Such $\eta\nu$ fermions and $s\nu$ fermions are non-interacting objects. Hence their energy is additive in the individual energies of the corresponding 2ν η-spinons and spinons,

respectively. For $U/4t > 0$ such quantum objects refer to the same occupancy configurations in terms of both rotated electrons and electrons.

---

[1] A. Damascelli, Z. Hussain, Z.-X. Shen, Rev. Mod. Phys. 75 (2003) 473.
[2] P. A. Lee, N. Nagaosa, X.-G. Wen, Rev. Mod. Phys. 78 (2006) 17.
[3] R. Coldea, S. M. Hayden, G. Aeppli, T. G. Perring, C. D. Frost, T. E. Mason, S.-W. Cheong, Z. Fisk, Phys. Rev. Lett. 86 (2001) 5377.
[4] J. M. P. Carmelo, S. Östlund, M. J. Sampaio, Ann. Phys. (2010), doi: 10.1016/j.aop.2010.03.002.
[5] E. H. Lieb, Phys. Rev. Lett. 62 (1989) 1201;
[6] C. N. Yang, S. C. Zhang, Mod. Phys. Lett. B 4 (1990) 759; S. C. Zhang, Phys. Rev. Lett. 65 (1990) 120.
[7] J. Stein, J. Stat. Phys. 88 (1997) 487.
[8] D. Jaksch, P. Zoller, Ann. Phys. 315 (2005) 52.
[9] R. Jördens, N. Strohmaier, K. Günter, H. Moritz, T. Esslinger, Nature 455 (2008) 204.
[10] A.-M. Daré, L. Raymond, G. Albinet, A.-M. S. Tremblay, Phys. Rev. B 76 (2007) 064402.
[11] C. N. Varney, C.-R. Lee, Z. J. Bai, S. Chiesa, M. Jarrell, R. T. Scalettar, Phys. Rev. B 80 (2009) 075116.
[12] J. M. P. Carmelo, arXiv:1003.4499.
[13] A. L. Chernyshev, D. Galanakis, P. Phillips, A. V. Rozhkov, A.-M. S. Tremblay, Phys. Rev. B 70 (2004) 235111.
[14] F. Kämpfer, M. Moser, U.-J. Wiese, Nucl. Phys. B 729 (2005) 317.
[15] E. H. Lieb, F. Y. Wu, Phys. Rev. Lett. 20 (1968) 1445.
[16] Minoru Takahashi, Progr. Theor. Phys 47 (1972) 69.
[17] M. J. Martins, P. B. Ramos, Nucl. Phys. B 522 (1998) 413.
[18] E. K. Sklyanin, L. A. Takhtadzhan, L. D. Faddeev, Theor. Math. Fiz. 40 (1979) 194.
[19] J. M. P. Carmelo, Nucl. Phys. B 824 (2010) 452.
[20] T. Senthil, Ashvin Vishwanath, Leon Balents, Subir Sachdev, Matthew P. A. Fisher, Science 303 (2004) 1490; T. Senthil, Leon Balents, Subir Sachdev, Ashvin Vishwanath, Matthew P. A. Fisher, Phys. Rev. B 70 (2004) 144407.
[21] Anders W. Sandvik, Phys. Rev. Lett. 98 (2007) 227202.
[22] Anders W. Sandvik, Phys. Rev. Lett. 104 (2010) 177201.
[23] J. E. Hirsch, Phys. Rev. B 31 (1985) 4403.
[24] P. Horsch, W. von der Linden, Z. Phys. B, 72 (1988) 181.
[25] A. W. Sandvik, Phys. Rev. B 56 (1997) 11 678.
[26] J. E. Hirsch, S. Tang, Phys. Rev. Lett. 62 (1989) 591.
[27] J. R. Schrieffer, X. G. Wen, S. C. Zhang, Phys. Rev. B 39 (1989) 11 663.
[28] S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis, J. E. Scalettar, Phys. Rev. B 40 (1989) 506.
[29] K. Borejsza, N. Dupuis, Phys. Rev. B 69 (2004) 085119.
[30] T. K. Kopeć, Phys. Rev. B 73 (2006) 132512.
[31] J. M. P. Carmelo, arXiv:0804.2379.
[32] J. M. P. Carmelo, K. Penc, J. Phys.: Cond. Matt. 18 (2006) 2881 and reference 8 therein.
[33] G. F. Giuliani, G. Vignale, Quantum theory of the electron liquid, Cambridge University Press, Cambridge, 2005.
[34] J. Falb, A. Muramatsu, Nucl. Phys. B 795 (2008) 519.
[35] N. D. Mermin, H. Wagner, Phys. Rev. Lett. 17 (1966) 1133.
[36] Stellan Östlund, Mats Granath, Phys. Rev. Lett. 96 (2006) 066404.
[37] P. W. Anderson, Phys. Rev. 86 (1952) 694.
[38] N. M. R. Peres, M. A. N. Araújo, Phys. Rev. B 65 (2002) 132404.
[39] M. Takahashi, J. Phys. C 10 (1977) 1289.
[40] P. M. Chaikin, T. C. Lubensky, Principles of Condensed Matter Physics, Cambridge University Press, Cambridge,1995.
[41] Nicolas Dupuis, private communication.
[42] P. Wiegmann, Phys. Rev. Lett. 60 (1988) 821; Nucl. Phys. B 323 (1989) 311.
[43] D. Pines, P. Nozières, in: The theory of quantum liquids, Benjamin, New York, 1996, Vol. 1.
[44] Y. R. Wang, Phys. Rev. B 46 (1992) 151.